Consequential LCA and LCC using linear programming: an illustrative example of biorefineries

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Abstract

Purpose This paper aims to demonstrate how LCA can be improved by the use of linear programming (LP) (i) to determine the optimal choice between new technologies, (ii) to identify the optimal region for supplying the feedstock, and (iii) to deal with multifunctional processes without specifying a certain main product. Furthermore, the contribution of LP in the context of consequential LCA and LCC is illustrated.

Methods We create a mixed integer linear program (MILP) for the environmental and economic assessment of new technologies. The model is applied in order to analyze two residual beech wood-based biorefinery concepts in Germany. In terms of the optimal consequences for the system under study, the principle of the program is to find a scaling vector that minimizes the life cycle impact indicator results of the system. We further transform the original linear program to extend the assessment by life cycle costing (LCC). Thereby, two multi-objective programming methods are used, weighted goal programming and epsilon constraint method.

Results and discussion The consequential case studies demonstrate the possibility to determine optimal locations of newly developed technologies. A high number of potential system modifications can be studied simultaneously without matrix inversion. The criteria for optimal choices are represented by the objective functions and the additional constraints such as the available feedstock in a region. By combining LCA and LCC targets within a multi-objective programming approach, it is possible to address environmental and economic trade-offs in consequential decision-making.

Conclusions This article shows that linear programming can be used to extend standard LCA in the field of technological choices. Additional consequential research questions can be addressed such as the determination of the optimal number of new production plants and the optimal regions for supplying the resources. The modifications of the program by additional profit requirements (LCC) into a goal program and Pareto optimization problem have been identified as promising steps toward a comprehensive multi-objective LCSA.

Keywords Eco-efficiency · Epsilon constraint · Goal programming · Mixed integer · Multi-objective optimization · Spatial LCA

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1 Introduction

Life cycle assessment (LCA), and in particular consequential LCA, is regarded as an appropriate tool for the assessment of environmental impacts of new bio-based technologies (e.g., Pawelzik et al. 2013). Despite the publication of various consequential modeling approaches, consequential LCA is still far from a proper systematization (Zamagni et al. 2012). Although the use of consequential and attributional LCA for decision-making is still being discussed (Ekvall et al. 2016; Hertwich 2014; Plevin et al. 2014), all approaches are based on the definition of consequential LCA that "is designed to generate information on the consequences of decisions" (Ekvall and Weidema 2004). Consequential LCA attempts to

determine how environmental flows will change due to the consequences of a decision (Curran et al. 2005). In contrast, attributional LCA focuses on describing the life cycle of a product by attributing the environmental flows to the product under study.

The choice for either determining consequences or attributional impacts also affects the way of modeling in terms of the multifunctional problem. This problem arises when a process provides more than one product that is not used within the system under study (Heijungs and Frischknecht 1998; Heijungs and Guinée 2007). In this case, the environmental burdens associated with the multifunctional process need to be allocated to different products. Several procedures have been developed to solve the multifunctional problem (Heijungs and Suh 2002). Consequential LCA approaches prefer to use substitution method to deal with the problem, whereas attributional LCA is a synonym for using the partitioning method (Ekvall and Weidema 2004; Thomassen et al. 2008; Schmidt 2010). The ISO standard suggests the expansion of the system as one method to deal with multifunctional unit processes (ISO 2006). Also, partitioning method is recommended, where dividing unit processes and expanding the product system cannot be avoided. Several authors have identified that system expansion is conceptually equivalent to substitution (Heijungs and Guinée 2007; Tillman et al. 1994). Thereby, the expansion of additional functions related to the co-products can either be carried out by subtracting the functions from the according process (substitution aka avoided burden method) or including the functions into the final demand vector (system expansion by expanding the functional unit). In any way, dealing with multifunctional processes by using partitioning and/or substitution method depends on a model choice (Majeau-Bettez et al. 2015). The choice of a certain model to deal with multifunctional processes is usually argued by the invertibility of the technology matrix (avoid rectangular matrix) and the argumentation that the model represents real world more closely than others would do (Suh et al. 2010). However, to solve systems with more products than processes (rectangular technology matrix), linear programming is a suitable way (Heijungs and Suh 2002).

A major issue for standard life cycle assessment, which addresses one state of a particular product system, might be the fact that no optimal production mixes can be determined. Usually, in LCA, this point is addressed by creating a small number of scenarios analyzing different product system alternatives iteratively (e.g., Budzinski and Nitzsche 2016; Renouf et al. 2018). However, such procedure can be very time-consuming. Particularly in consequential LCA, this could be an issue. In many cases, not only the consequences of a potential decision need to be described, but rather the optimal decision itself shall be identified. To overcome limitations in LCA, among other methods such as fuzzy programming (Tan et al. 2008) or graph methods (Vance et al. 2015), the combined use

of LCA with linear programming (LP) has a longer tradition. Azapagic and Clift (1995, 1998) introduced LP in the field of process engineering. Thereby, LP is used to allocate environmental burdens to multiple co-products by means of the marginal values at the solution of the LP model. Recent studies exist in the field of biomass utilization. Vadenbo et al. (2017) used a multi-objective optimization model to determine the optimal activity levels of a set of biomass process options. Kostin et al. (2012) carried out an assessment with a mixed-integer linear programming approach for ethanol production chains. Based on a rectangular choice-of-technology model (Duchin and Levine 2011), Kätelhön et al. (2016) built a technology choice model (TCM) for consequential LCA of rice production. Despite the attempts to incorporate LCA into a consistent multi-objective framework combining linear programming and life cycle sustainability assessment (LCSA) (e.g., Gong and You 2017; Steubing et al. 2011; Liu et al. 2010), a conceptual discussion on how consequential LCA and LCC can be extended by LP is still scarce.

The aim of this paper is, hence, to demonstrate how LCA can be extended by the use of linear programming (i) to determine the optimal choice between new technologies, (ii) to identify the optimal region for supplying the feedstock, and (iii) to deal with multifunctional processes without specifying a certain main product. In doing so, we use the matrix-based notation of Heijungs and Suh (2002) and create a rectangular mixed integer linear program and carry out a case study to illustrate its applicability. Thereby, two wood-based biorefinery concepts are analyzed in terms of the optimal consequences for the total system under study. Furthermore, we modify the original linear program into a weighted goal programming problem and a Pareto optimization model those extend the environmental focus on sustainability by adding the economic perspective through a life cycle costing (LCC) approach.

2 Computational structure of LCA and LCC

The computational structure of LCA is comprehensively described by Heijungs and Suh (2002). Mathematically, the first step of life cycle inventory (LCI) analysis is the determination of the scaling vector **s.** The components of this vector scale processes of a system up or down such that the output of unit processes exactly matches the final demand. The final demand vector **f** includes the reference flows r, which are defined within the goal and scope of a LCA study. The scaling vector can be determined by the multiplication of the inverse of technology matrix **A** with the final demand vector.

$$s = A^{-1} f, \text{ with } f_i = \begin{cases} > 0 \text{ if } i \in r \\ 0 \text{ otherwise} \end{cases} \quad (1)$$

The next step of the LCI analysis is to specify the inventory vector **g** according to the reference flows. This is done by multiplying the intervention matrix **B** with the scaling vector.

$$\mathbf{g} = \mathbf{Bs} \qquad (2)$$

Life cycle impact assessment (LCIA) transforms the interventions into more understandable impact indicator results. The impact vector **h** can be calculated by multiplying the matrix of characterization factors **Q** with the inventory vector.

$$\mathbf{h} = \mathbf{Qg} \qquad (3)$$

The so-called multifunctional problem arises if a process generates more than one product and if and only if the delivered functions are not used in the same proportion in the system (Heijungs and Frischknecht 1998). The most common approaches to solve the multifunction problem can be classified into partitioning method and substitution method (Heijungs and Guinée 2007). By applying these procedures, the technology matrix **A** becomes square, since an equal amount of rows and columns exists. The partitioning method divides the multifunctional process into processes that are mono-functional by the use of allocation factors. Several ways to gain these factors are possible, e.g., due to physical or monetary characteristics of the products. The substitution method requires the definition of a mono-functional process, which provides the avoided product to the multi-functional process. Adding this process to the technology matrix **A** makes its inversion possible.

An interesting but not often recognized characteristic of LCA is the existence of a price model beside the quantity model ($\mathbf{As} = \mathbf{f}$), which is similar to input-output models. This becomes obvious when a price vector $\boldsymbol{\alpha}$ is introduced (cf. Heijungs et al. 2013). Using this price vector, it is possible to compute the value added v per process.

$$\mathbf{v} = \mathbf{A}'\boldsymbol{\alpha} \qquad (4)$$

To determine the value added in terms of a reference flow, the elements of the scaling vector **s** can be multiplied by the value added of the corresponding processes, where **1** is the summation operator (vector of ones).

$$\mathbf{v}'_{scaled} = \mathbf{1}\left(diag\left(\mathbf{v}'\right)\mathbf{s}\right) \qquad (5)$$

This value added vector can then be used to determine life cycle costs (LCC). Heijungs et al. (2013) define life cycle cost of a composite final demand as $l = \sum_j -v_j^{scaled}$, where j runs over all case such that technical coefficient $a_{ij} > 0$, where reference flows i is such that $f_i \neq 0$. In other words, the life cycle costs of reference flows, which are specified in the final demand vector, are the negative sum of the corresponding entries in the scaled value added vector.

3 Exemplary case study

In the following sections, we demonstrate how the previously mentioned equations can be modified to create a rectangular choice-of-technology model in regard to the goal and scope of the study (Sect. 3.1). Therefore, we define a mixed integer linear program (Sect. 3.2) and determine the results of an exemplary case study (Sect. 3.3). To include LCC aspects, we transform the original problem into a weighted goal programming problem and a Pareto optimization model in Sects. 3.4 and 3.5, respectively.

3.1 Goal and scope

The study concerns two exemplary biorefinery concepts. The concepts and data are based on Budzinski and Nitzsche (2016). The first biorefinery concept produces ethylene, organosolv lignin, and biomethane. The second configuration produces the same products as the first one except for ethylene that is replaced by ethanol. The annually produced amounts of the multifunctional biorefinery processes are illustrated in Table 1. The goal of the exemplary case study is threefold. Firstly, we want to determine the biorefinery that is more appropriate to reduce environmental impacts in regard to the current production system. Secondly, we want to determine at which site the biorefineries should be located (Fig. 1). And finally, to identify districts for supplying woody biomass feedstocks.

Table 1 Annual input and output of biorefinery processes

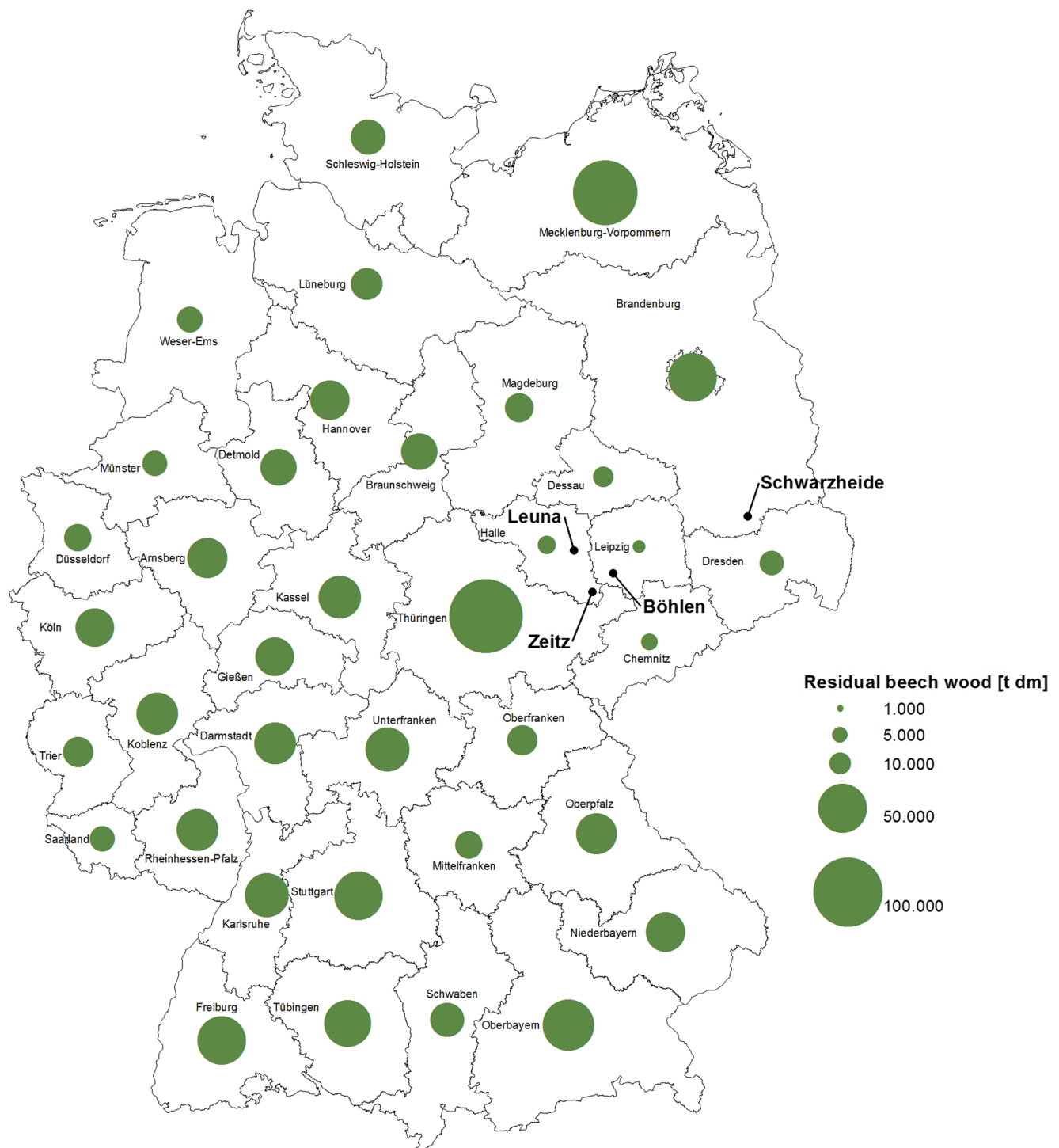|	Biorefinery 1	Biorefinery 2
Biomethane (m^3)	$5.05 \cdot 10^7$	$5.05 \cdot 10^7$
Ethylene (kg)	$4.14 \cdot 10^7$	0
Hydrolysis lignin (MJ)	$1.96 \cdot 10^9$	$1.96 \cdot 10^9$
Ethanol (MJ)	0	$1.87 \cdot 10^9$
Organosolv lignin (kg)	$6.22 \cdot 10^7$	$6.22 \cdot 10^7$
Sodium hydroxide (kg)	$-5.04 \cdot 10^5$	$-5.04 \cdot 10^5$
Magnesium sulfate (kg)	$-3.57 \cdot 10^5$	$-3.57 \cdot 10^5$
Phosphorus (kg)	$-3.57 \cdot 10^5$	$-3.57 \cdot 10^5$
Sulfur (kg)	$-3.57 \cdot 10^5$	$-3.57 \cdot 10^5$
Sulfuric acid (kg)	$-3.76 \cdot 10^6$	$-3.76 \cdot 10^6$
Fodder yeast (kg)	$-2.32 \cdot 10^6$	$-2.32 \cdot 10^6$
Lime, packed (kg)	$-3.84 \cdot 10^4$	$-3.84 \cdot 10^4$
Refrigerant (kg)	$-4.94 \cdot 10^4$	0
Heat, natural gas (MJ)	$-5.86 \cdot 10^7$	0
Electricity, natural gas (kWh)	$-1.08 \cdot 10^9$	$-1.35 \cdot 10^9$
Chemical factory (unit)	$-1.05 \cdot 10^8$	$-9.52 \cdot 10^7$
Treated wastewater (m^3)	$-3.33 \cdot 10^{-2}$	$-3.33 \cdot 10^{-2}$
Water (kg)	$-2.84 \cdot 10^6$	$-3.16 \cdot 10^6$
Beech wood (kg dm)	$-4.00 \cdot 10^8$	$-4.00 \cdot 10^8$

Fig. 1 Potential location for the two biorefinery types and annual availability of residual beech wood from forests within German districts (scenario 100%)

For simplicity reasons, we focus on four chemical parks of the Central European Chemical Network[1] as potential plant locations, which would in principal allow the building of the two biorefinery concepts: Leuna, Böhlen, Zeitz, and Schwarzheide. We assume that all chemical parks can provide the required infrastructure and utilities in the same manner. Furthermore, we suppose that either one or none of the biorefinery concepts can be built at a location. Data on residual beech wood are estimated at the level of 37 administrative districts in Germany according to Polley and Kroiher (2006).

This residual wood is currently not used and remains in forests after chopping, which might be possibly used as feedstock for biorefineries without inducing feedstock rivalry (Michels 2009). Since the 100% use of available beech wood residuals is quite optimistic, we introduce a second scenario in which the availability in each region is reduced by 50% (cf. Michels 2009). The transport distances from the districts to the four potential plant locations can be covered by train and/or truck. In this study, we assume that up to 200 km, the wood is transported only by truck. For distances greater than 200 km, the wood is additionally transported by train. Thereby, we further assume that a minimal distance (between 10 and 30 km depending on the availability of train network) is covered by truck. Varying transport distances for other pre-products of the biorefineries are neglected.

We assume that the new biorefinery products compete with existing products of the current system. Hence, we define *substitutable* reference products for each biorefinery product: biomethane vs. natural gas, bio-based ethylene vs. fossil ethylene, hydrolysis lignin vs. lignite briquettes, ethanol vs. petrol, and organosolv lignin vs. polyol. The definition of these avoided products is a long-discussed issue in LCA. Since the general societal aim is to move towards a bio-based economy, we use fossil-based references that provide the same functions.

The amounts of reference flows are specified in regard to the German demand of these products within the current system. Thereby, the reference flows need to be specified in the manner that the products of current processes must provide the same functions as of the biorefinery products. In the example, we assume that this is guaranteed, e.g., by referring to MJ in the case of ethanol and gasoline.

For LCIA, we chose the category climate change taking into account the three substances CO_2, CH_4, and N_2O.

3.2 The linear programming model

According to Heijungs and Suh (2002), the principle of extending LCA by LP is to relax the balance equations into inequations. Hence, we can replace the equation

$$\mathbf{As} = \mathbf{f} \tag{6}$$

by the inequation

$$\mathbf{As} \geq \mathbf{f}. \tag{7}$$

By using this formulation, the solution of such program would allow flows that are greater than those specified in the final demand vector. Regarding the special case in which processes are defined to be strictly mono-functional, the formulation as $\mathbf{As} = \mathbf{f}$ would also work for solving the LP. The formulation in Eq. (7) also provides solutions for cases in which

multi-output processes are considered in the upstream system and, hence, is more general.

The overall program can be summarized by the formulas 8 to 11 considering that the scaling factors of biorefinery processes $s_1, s_2, s_3, s_4, s_5, s_6, s_7$, and s_8 are integers. Thereby, Eq. 8 represents the objective function of minimizing environmental impacts. Equation 9 illustrates the system under study including all potential biorefineries, feedstock regions, and transportation alternatives. Equation 10 includes the capacity constraints for feedstock availability in the regions. Equation 11 considers the fact that only one of the two biorefinery options can be built at a potential location. By using the linear programming model, we are interested in the reduction of the total environmental impacts of the current system. Hence, the objective function results from Eqs. 2 and 3, and the target is to find a vector $\mathbf{s}$ that minimizes the total impacts h of the system, which is expressed by matrix $\mathbf{A}$. A visualization of the modeling principle including the sub-matrices of $\mathbf{A}$ is given in Fig. 2. The fundamental principle of the model is to check whether environmental impacts can be reduced by biorefinery 1 or 2 considering 4 potential locations ($\mathbf{A}_{BRS}$) and 37 regions of wood supply ($\mathbf{A}_S$). If not, the model would only choose current processes ($\mathbf{A}_{Ref}$) to provide the components of the final demand.

$$\text{Minimize } h = \mathbf{QBs} \tag{8}$$

subject to

$$\mathbf{As} \begin{cases} \geq f_i > 0 & \text{if } i \in r \\ = f_i = 0 & \text{if } i \in T, S \\ \geq f_i = 0 & \text{otherwise} \end{cases} \tag{9}$$

$$\mathbf{0} \leq \mathbf{s} \leq \mathbf{c} \tag{10}$$

$$\begin{aligned} s_1 + s_2 &\leq 1 \\ s_3 + s_4 &\leq 1 \\ s_5 + s_6 &\leq 1 \\ s_7 + s_8 &\leq 1 \end{aligned} \tag{11}$$

with $s_1, s_2, s_3, s_4, s_5, s_6, s_7, s_8 \in \mathbb{N}$

The rectangular technology matrix $\mathbf{A}$ with the dimension of products-by-processes consists of several sub-matrices.

$$\mathbf{A} = \begin{bmatrix} \mathbf{A}_{BRS} & 0 & 0 & 0 & \mathbf{A}_{Ref} \\ -\mathbf{A}_{up}^* & \mathbf{A}_{up} & -\mathbf{A}_{up}^{**} & -\mathbf{A}_{up}^{***} & 0 \\ 0 & 0 & \mathbf{A}_S & -\mathbf{A}_S^* & 0 \\ -\mathbf{A}_T^* & 0 & 0 & \mathbf{A}_T & 0 \end{bmatrix} \tag{12}$$

These sub-matrices have the following dimensions:

$\mathbf{A}_{BRS}$ $i_r \times j_{BRS}$ (5×8)
$\mathbf{A}_{Ref}$ $i_r \times j_{Ref}$ (5×5)
$\mathbf{A}_{up}$ $i_{up} \times j_{up}$ (17×17)
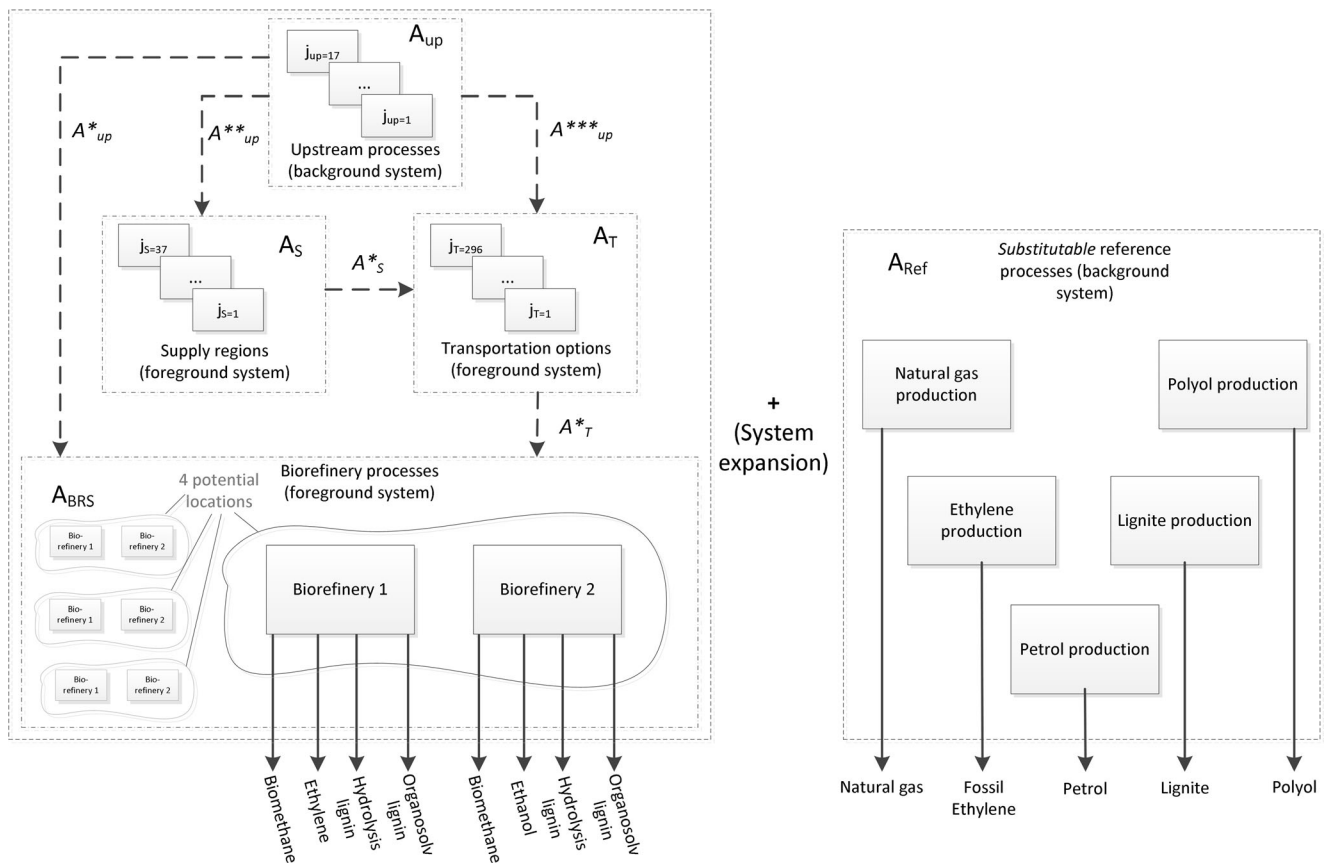
Fig. 2 Simplified flowchart

$-\mathbf{A}_{up}^{*}$	$i_{up} \times j_{BRS}$ (17 × 8)
$-\mathbf{A}_{up}^{**}$	$i_{up} \times j_{S}$ (17 × 37)
$-\mathbf{A}_{up}^{***}$	$i_{up} \times j_{T}$ (17 × 296)
$-\mathbf{A}_{T}^{*}$	$i_{T} \times j_{BRS}$ (8 × 8)
$\mathbf{A}_{T}$	$i_{T} \times j_{T}$ (8 × 296)
$-\mathbf{A}_{S}^{*}$	$i_{S} \times j_{T}$ (37 × 296)
$\mathbf{A}_{S}$	$i_{S} \times j_{S}$ (37 × 37).

with,

i_{r}	biorefinery/reference product
i_{up}	product of upstream process
i_{T}	transported wood
i_{S}	supplied wood in a district
j_{BRS}	biorefinery process
j_{Ref}	substitutable reference process
j_{up}	upstream process
j_{S}	region for supplying wood
j_{T}	transport option

The columns of matrix $\mathbf{A}_{BRS}$ represent the biorefinery options j_{BRS} of each type at each potential location. The rows of this matrix represent the products i_{r} which can also be produced by current reference processes j_{Ref}. Matrix $\mathbf{A}_{Ref}$ includes current available processes j_{Ref} that produce the same functions i_{r} as the biorefinery processes.

To address the choice for a certain district, which deliver the residual beech wood, the model is extended by the matrices $\mathbf{A}_{T}$, $-\mathbf{A}_{T}^{*}$, $\mathbf{A}_{S}$ and $-\mathbf{A}_{S}^{*}$. Matrix $\mathbf{A}_{S}$ is an identity matrix to consider the different alternatives of beech wood supply from the 37 districts. Matrices $-\mathbf{A}_{S}^{*}$ and $\mathbf{A}_{T}$ are needed to include the alternatives of beech wood transport from each district to each one of the 8 biorefinery alternatives. The linkage of the these alternatives to the biorefinery options is represented by matrix $-\mathbf{A}_{T}^{*}$.

Upstream processes in matrix $\mathbf{A}_{up}$, which are needed to provide the pre-products of the biorefineries, the cultivation, and transportation of wood and the reference products, complete the rectangular $\mathbf{A}$ matrix.

The program is designed as an LCA for a final demand f_{r} on reference flows r, which are characterized by the products of the biorefinery system and the corresponding reference products (biomethane/natural gas, bio-based ethylene/fossil ethylene, hydrolysis lignin/lignite briquettes, ethanol/petrol, organosolv lignin/polyol). The amounts for the multiple components of the functional unit are taken from statistical sources (e.g., VCI 2018; SDK 2017) and represent those of a current German demand. Other components of the final demand

vector **f** are set to zero. The design of an LCA for a demand on the functional unit does not take into account the linkage of downstream processing with the modeled upstream processing so that economy-wide impacts are cut off (Suh 2004). However, the modeling in regard to the functional unit is a general principle of LCA (Peters and Hertwich 2006). To ensure the balance between supply and demand of transported beech wood, the constraint $\begin{bmatrix} 0 & 0 & \mathbf{A}_S & -\mathbf{A}_S^* & 0 \\ -\mathbf{A}_T^* & 0 & 0 & \mathbf{A}_T & 0 \end{bmatrix} \mathbf{s} = f_{S,T} = 0$ is introduced.

We further define the first eight scaling factors for the biorefinery processes to be integers. This choice is necessary, since the data collection for the biorefineries is based on process simulation for a specific capacity. The intermediate flows and environmental interventions associated with this capacity are not up- or downscalable in a linear manner. The program is completed by introducing lower bounds (set to 0) and a vector of upper bounds **c**. In regard to the availability of residual beech wood in each district, the data of Fig. 1 is considered as upper bounds for s_{j_S}. The upper bounds **c** for the scaling factors of biorefinery processes ($s_{j_{BRS}}$) were set to 1, since we assume that only one biorefinery can be built at a chemical park.

The LCI data for upstream biorefienry processes and for the *substitutable* reference system is taken from the ecoinvent 3.2 database (cut-off model). The whole problem and the corresponding data can be studied in more detail in the Electronic Supplementary Material (MILP_LCA.xlsx).

3.3 Results

To solve the mixed integer linear program, the intlinprog solver in Matlab was used. An additional scenario is analyzed in which the available amount of beech wood is reduced by 50%. The results for 100% scenario (1.14 Mt dm beech wood in Germany) indicate that two biorefineries with a capacity of 0.4 Mt dm are built at the considered chemical parks. Since the scaling factors for biorefineries are defined as integers, not the total available amount of beech wood is exhausted. The optimal locations to build the biorefineries are Zeitz and Schwarzheide. It is visible that for both scenarios, the ethylene-producing biorefinery 1 is more preferable to reduce greenhouse gas emissions than the ethanol-producing biorefinery 2 (Table 2). When reducing the available residual wood for all districts by 50%, another location becomes more preferable than those of the 100% scenario. This is an interesting result, since one might assume that one of the locations identified in the 50%

would be chosen. The total reduction of the impacts on climate change compared to the impacts of the current system ($\mathbf{h}_{Ref} = \mathbf{Q}_{Ref} \cdot \mathbf{B}_{Ref} \cdot \mathbf{A}_{Ref}^{-1} \cdot f_r$) is 4.76 Mt/a CO_2 eq. in the 100% scenario and 2.38 Mt/a CO_2 eq. in the 50% scenario.

The contribution analysis for the 100% scenario shows that current *substitutable* processes still provide the major part of the overall GHG emissions (lignite production 88.48%, natural gas production 8.24%, petrol production 1.95%, ethylene production 1.05%, polyol production 0.25%) whereas the biorefinery system plays a minor part (biorefineries 0.12%, wood production −0.20%, other upstream processes including transport 0.12%). Due to the feedstock availability of German beech wood residuals, only a small ratio of current GHG emissions could be reduced. Detailed information on contribution analyses is provided in the Electronic Supplementary Material (MILP_LCA.xlsx).

To study the origin of wood supply it is possible to analyze the corresponding scaling factors of the transport processes j_T. These factors represent the contribution to the overall wood demand of the biorefineries. Figure 3a illustrates the solutions for the 100% scenario. Thereby, the biorefinery in Zeitz is delivered from regions in the middle west of Germany and from regions in the middle south. In contrast, the biorefinery in Schwarzheide is delivered by regions in the northeastern part of Germany.

Due to the reduced wood availability in the 50% scenario, regions supplying the feedstock to biorefinery 1 in Leuna are distributed throughout Germany (Fig. 3b). Hence, a large catchment area is required to fulfill the demand of the biorefinery in the scenario with reduced residual beech wood availability.

3.4 Inclusion of LCC by multi-objective optimization

Since we have not considered transportation and other costs so far in this case study, we adopt the model by introducing an additional objective for life cycle costing. In doing so, we introduce for the specific biorefineries an additional input factor matrix **F** with subcategories k (expressed in monetary units): personal costs, taxes, insurance, and administration. As Heijungs et al. (2013) showed, the consideration of costs for the inputs and outputs of the processes of the technology matrix **A** can be carried out by using a price vector α. Since we focus on the investor's perspective, price information is only required for products that are relevant for the profitability of the biorefineries. The additional objective function, which includes costs for processed and produced commodities of the biorefinery processes as well as the costs for transported beech wood, can be derived as

Table 2 Results of the mixed integer linear program, per annum

	100% scenario	50% scenario
Biorefinery 1, Leuna (pc.)	0	1
Biorefinery 2, Leuna (pc.)	0	0
Biorefinery 1, Zeitz (pc.)	1	0
Biorefinery 2, Zeitz (pc.)	0	0
Biorefinery 1, Böhlen (pc.)	0	0
Biorefinery 2, Böhlen (pc.)	0	0
Biorefinery 1, Schwarzheide (pc.)	1	0
Biorefinery 2, Schwarzheide (pc.)	0	0
Natural gas (m^3)	$9.580053 \cdot 10^{10}$	$9.585027 \cdot 10^{10}$
Fossil ethylene (kg)	$5.017197 \cdot 10^{9}$	$5.058598e \cdot 10^{9}$
Lignite (MJ)	$3.214008 \cdot 10^{13}$	$3.214204 \cdot 10^{13}$
Petrol (MJ)	$7.340000 \cdot 10^{11}$	$7.340000 \cdot 10^{11}$
Polyol (kg)	$4.342704 \cdot 10^{8}$	$4.964352 \cdot 10^{8}$
h (kg CO_2-eq.)	$7.152422 \cdot 10^{11}$	$7.156019 \cdot 10^{11}$
Potential savings $h - h_{Ref}$ (kg CO_2-eq.)	$-7.193181 \cdot 10^{8}$	$-3.596181 \cdot 10^{8}$

$$Maximize\ z = \sum_{j_{BRS}=1}^{J_{BRS}} \left(\left(\sum_{i_{BRS}=1}^{I_{BRS}} A_{i_{BRS},j_{BRS}}^{BRS} \cdot \alpha_{i_{BRS}} \right) - \left(\sum_{i_{up}=1}^{I_{up}} A_{i_{up},j_{BRS}}^{*} \cdot \alpha_{i_{up}} \right) - \left(\sum_{i_T=1}^{I_T} A_{i_T,j_{BRS}}^{*} \cdot \alpha_{i_T} \right) - \sum_{k=1}^{K} F_{k j_{BRS}} \right)$$

$$\cdot s_{j_{BRS}} - \sum_{j_T=1}^{J_T} \left(\sum_{i_{up}=1}^{I_{up}} A_{i_{up},j_T}^{***} \cdot \alpha_{i_{up}} \right) \cdot s_{j_T} \tag{13}$$
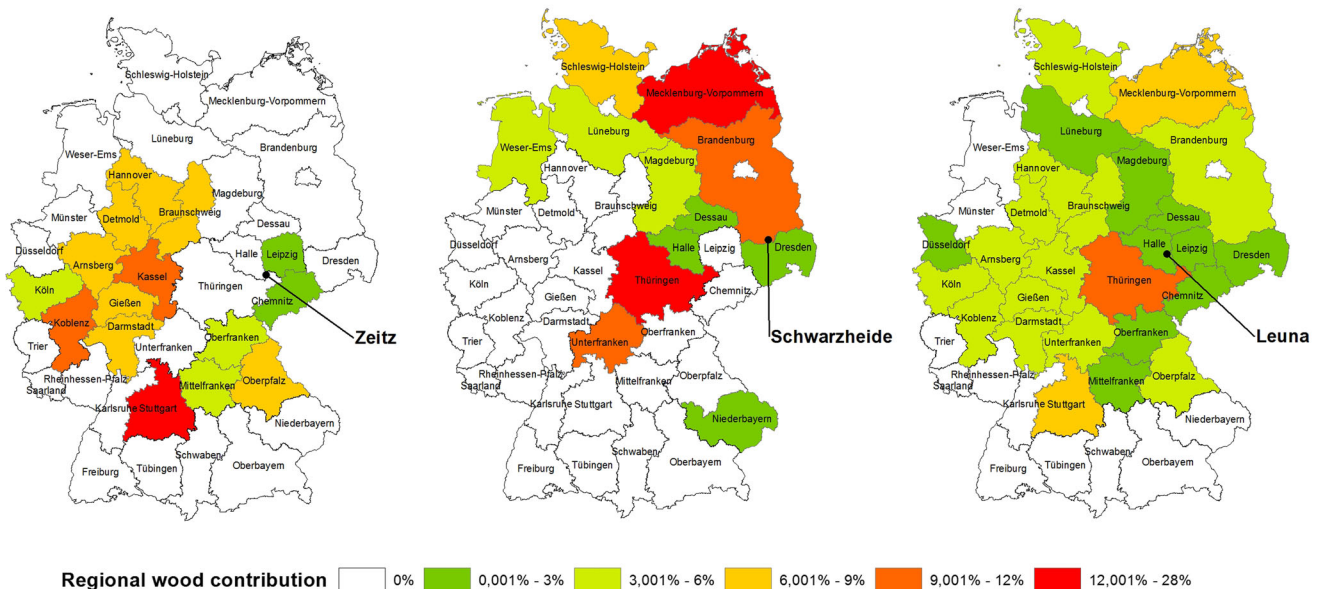

Fig. 3 Optimal regions to supply beech wood to the biorefineries

Equation 13 consists of two major terms. The first term considers the cash-flows related directly to the biorefinery processes j_{BRS} including revenues for biorefinery products ($\sum_{i_{BRS}=1}^{I_{BRS}} A^{BRS}_{i_{BRS},j_{BRS}} \cdot \alpha_{i_{BRS}}$), payments for pre-products ($\sum_{i_{up}=1}^{I_{up}} A^*_{i_{up},j_{BRS}} \cdot \alpha_{i_{up}}$), payments for wood ($\sum_{i_T=1}^{I_T} A^*_{i_T,j_{BRS}} \cdot \alpha_{i_T}$), and other payments such as for personal and insurance ($\sum_{k=1}^{K} F_{kj_{BRS}}$). The second term represents the payments related to the transportation options j_T of wood. This expression can be simplified in matrix notation as

$$Maximize\ z = \mathbf{p\ddot{E}s}, \tag{14}$$

where the components of vector $\mathbf{p}$ specify the profit of processes j.

This LCC approach is congruent to the proposed one by Heijungs et al. (2013), but differs in the way that only those costs are taken into account, which are relevant for the investment decision for the biorefinery options. This choice is concerned with taking the view of potential investors maximizing the profit of a biorefinery. Thereby, only the costs are considered that are relevant for the decision on the profitability of the biorefinery (including costs for transportation and additional inputs). Besides to this simple LCC approach, however, there are further possibilities to consider cost information by the model. For example, it might also reasonable to explicitly take into account the profit for reference processes competing with biorefineries, or to use discounted cash flow analysis taking into account the time value of money (e.g., net present value). However, additional data must be collected. For simplicity reasons, we chose the standard approach of LCC in this study.

To deal with multiple objectives in linear programming, basically, three groups can be distinguished: a priori, interactive, and a posteriori methods (Hwang and Masud 1979). The first class requires the definition of preferences between goals at the beginning of the solution process. The latter class requires the prioritization at the end after the presentation of all Pareto optimal solutions. To illustrate the pros and cons of the broad range of applications, we modify the linear program in the next sections choosing weighted goal programming for an a priori approach and epsilon-constraint method for a posteriori approach.

3.4.1 Goal programming

In weighted goal programming, the objectives are taken explicitly into account as constraints (Miller and Blair 2009). The principle of goal programming (GP) is to use slack variables d_h and d_z that measure the deviation from the desired environmental and economic target values h and z,

respectively. The target function of the goal program minimizes the deviations in terms of the desired values. For h, we chose 0, since the aim of a sustainable economy can be regarded to be carbon neutral. For the profit target z, we choose an arbitrarily large value (1.00E + 15 €) which is equivalent to maximize the objective function. The weighting factors w result in a normalization and prioritization of the target deviations. For greenhouse gas emissions, we use the weighting factor $w_h = 0.025$ which is the value of expected damage costs in terms of €/kg CO_2-eq (De Bruyn et al. 2010). The choice of this factor is concerned by uncertainty, comparable to those related to the monetization of environmental impacts. Due to the illustrative character of this study, we do not assess this in detail. However, robust optimization may take uncertainty of parameters explicitly into consideration (Wang and Work 2014). The weighting factor w_z is set to 1, since the unit of the profit target is €.

$$Minimize\ \mathrm{w}_h d_h^+ + \mathrm{w}_z d_z^- \tag{15}$$

subject to

$$\mathbf{As} \begin{cases} \geq f_i > 0 & \text{if } i \in r \\ = f_i = 0 & \text{if } i \in t \\ \geq f_i = 0 & \text{otherwise} \end{cases} \tag{16}$$

$$\mathbf{QBs} + \mathrm{d}^- - \mathrm{d}^+ = \mathrm{h} \tag{17}$$

$$\mathbf{ps} + \mathrm{d}^- - \mathrm{d}^+ = \mathrm{z} \tag{18}$$

$$\mathbf{0} \leq \mathbf{s} \leq \mathbf{c} \tag{19}$$

$$\begin{aligned} s_1 + s_2 &\leq 1 \\ s_3 + s_4 &\leq 1 \\ s_5 + s_6 &\leq 1 \\ s_7 + s_8 &\leq 1 \end{aligned} \tag{20}$$

with $s_1, s_2, s_3, s_4, s_5, s_6, s_7, s_8 \in \mathbb{Z}$

Table 3 shows the result of the GP model for both scenarios. Contrary to the LP model, the optimal solution is the ethanol concept (biorefinery 2) for both scenarios. The optimal chemical parks of the chosen biorefineries are identical to those of the LP model. The regions that deliver the wood feedstock to the plants are also identical. Therefore we omit to illustrate them again in the map. The reason for choosing biorefinery 2 is the higher priority to minimize the negative distance to the economic target value (d_z^-) compared to the priority of minimizing the positive distance to the environmental target value (d_h^+). Thus, the total annual amount of environmental savings is reduced from 0.72 Mt/a and 0.36 Mt/a CO_2-eq to 0.37 Mt/a and 0.18 Mt/a CO_2-eq in the 100%

Table 3 Results of the goal program, per annum

	100% scenario	50% scenario
Biorefinery 1, Leuna (pc.)	0	0
Biorefinery 2, Leuna (pc.)	0	1
Biorefinery 1, Zeitz (pc.)	0	0
Biorefinery 2, Zeitz (pc.)	1	0
Biorefinery 1, Böhlen (pc.)	0	0
Biorefinery 2, Böhlen (pc.)	0	0
Biorefinery 1, Schwarzheide (pc.)	0	0
Biorefinery 2, Schwarzheide (pc.)	1	0
d_h^+ (kg CO_2-eq.)	$7.155941 \cdot 10^{11}$	$7.157785 \cdot 10^{11}$
d_z^- (€)	$9.999991 \cdot 10^{13}$	$9.999995 \cdot 10^{13}$
Profit $z - d_z^-$ (€)	$9.174736 \cdot 10^7$	$4.509840 \cdot 10^7$
Potential savings $h_{RefS} - d_h^+$ (kg CO_2-eq.)	$-3.674181 \cdot 10^8$	$-1.830181 \cdot 10^8$

scenario and the 50% scenario, respectively. The annual profits are 92 Mio € and 45 Mio € in the 100% scenario and the 50% scenario, respectively. When introducing economic aspects, this result is similar to the one of Budzinski and Nitzsche (2016) who also concluded that the ethanol-producing concept has a better economic performance than the ethylene-producing concept. However, in Budzinski and Nitzsche (2016), only the ethanol biorefinery is profitable, which is contrary to the results of this study. The reason for that is the authors' use of a dynamic cost calculation approach that takes the time value of money into account. Thereby, the internal rate of return on the investment must be at least equal the minimum rate of return a decision-maker is willing to accept. The time value of money usually is not considered in

process-based LCC. However, a possible way is to implement an additional constraint in the LP model that ensures the exceeding of a minimal positive profit value.

3.4.2 Epsilon-constraint method

A disadvantage of goal programming might be the requirement of defining of preferences at the beginning of the solution process. Alternatively, a posteriori methods are available to prioritize between goals after the generation of all Pareto efficient solution. In doing so, epsilon-constraint method has been already used in the field of LCA (e.g., Azapagic and Clift 1999). Here, in this study, we apply the epsilon-constraint method in GAMS (Mavrotas 2009a, b). Thereby, the target

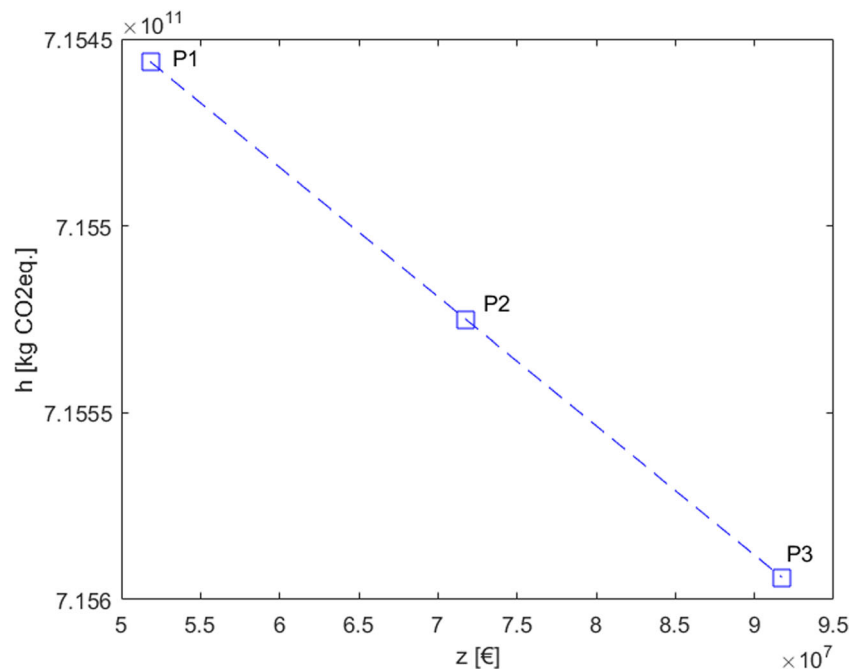**Fig. 4** Pareto front (100% scenario). h: environmental impacts; z: profit

Table 4 Results of the epsilon-constraint method (100% scenario), per annum

	P1	P2		P3
h (kg CO_2-eq.)	$7.154561 \cdot 10^{11}$	$7.155251 \cdot 10^{11}$		$7.155941 \cdot 10^{11}$
z (€)	$5.183191 \cdot 10^{7}$	$7.178963 \cdot 10^{7}$		$9.174736 \cdot 10^{7}$
		a)	b)	
Biorefinery 1, Leuna (pc.)	0	0	0	0
Biorefinery 2, Leuna (pc.)	0	0	0	0
Biorefinery 1, Zeitz (pc.)	1	0	1	0
Biorefinery 2, Zeitz (pc.)	0	1	0	1
Biorefinery 1, Böhlen (pc.)	0	0	0	0
Biorefinery 2, Böhlen (pc.)	0	0	0	0
Biorefinery 1, Schwarzheide (pc.)	1	1	0	0
Biorefinery 2, Schwarzheide (pc.)	0	0	1	1

function of profit (Eq. 14) is additionally involved in the optimization problem as

$$Minimize \ (h(s), -z(s)). \qquad (21)$$

Pareto optimal solutions are solutions that cannot be improved in any of the two objectives without degrading the other objective. The Pareto optimal solutions of the 100% scenario are illustrated in Fig. 4. In this example, three Pareto optimal solutions are identified. The dominated solutions, which are not Pareto optimal, are below the blue line. However, more comprehensive problems can result in various non-dominated solutions. Solution P1 suggests biorefinery 1 (ethylene) in Zeitz and in Schwarzheide. In contrast to this environmentally most preferable solution, P3 contains the most preferable solution in terms of profit (Table 4). Thereby, biorefinery 2 (ethanol) is located in Zeitz and Schwarzheide. The solution P2 can be interpreted as a compromise between these extreme solutions of maximal profit and minimal impacts on climate change. Furthermore, the solution may become worthwhile due to the fact that both biorefinery concepts (ethylene and ethanol) would be built in Zeitz and Schwarzheide. This mixture of technologies might be also interesting for decision-making. In contrast to goal programming in which only one solution is determined in accordance with the a priori defined priority order, Pareto optimization allows the decision-maker to deal with trade-offs after investigating the non-dominated solutions.

The non-dominated solutions of the 50% scenario are illustrated in Fig. 5. The most beneficial solution P1 in terms of impacts on climate change is given by the biorefinery 1 located in Leuna. Biorefinery 2 in Leuna is the most profitable solution P3. Contrary to the 100% scenario, the compromise solution P2 is near to P3 suggesting biorefinery 2 in Böhlen. An interesting fact is that P3 (in both scenarios) is the solution of the goal programming approach (Sect. 3.4.1). However, the identification of all non-dominated solutions, even if the

solution is nearly located to another such as P2 in the 50% scenario, clearly is an advantage of a posteriori approaches over a priori methods.

A special look requires the influence of transportation distances on the overall result (profit and environmental impacts). In this study the transportation of feedstock only has a limited influence on the overall profit of the biorefinery. For instance, the difference between biorefinery type 2 in Leuna compared to the location in Böhlen is 177,280 € per year (Table 5). In regard to the potential reduction of GHG emissions, the difference is even less significant. Here, the biorefinery 2 in Leuna has a reduction potential at 2000 kg CO_2 eq. per year higher than in Böhlen (Pareto point 2 and 3 of 50% scenario, Table 5). Comparing this difference with the overall GHG emissions of the system, one might assume that the results are not reliable in terms of data inaccuracies. To address this point, we have a look at the reference flows of the final demand vector. The chosen amounts represent an estimated total demand for Germany and, hence, are quite high. However, lower values would not lead to different results and would not reduce uncertainty. In fact, the choice of values for the considered reference flows is arbitrary. The determination of optimal locations for biorefineries is, hence, not affected by this choice. Since we here assume identical conditions at the potential chemical parks, the identification of optimal locations is only determined by the transport distances and the corresponding impacts and costs. On the contrary, the choice for the type of biorefinery in terms of environmental impacts is mainly dominated by its emissions and those of the reference processes. In terms of profit, the optimal solution is mainly dominated by the corresponding costs for biorefinery (pre)-products. In conclusion, the results for the optimal choices of locations for biorefineries may be considered being robust in the face of data uncertainties in other parts of the model. A problem that might result is numerical issues when solving a problem with large discrepancies in order of

magnitude. Back substituting the solution vectors **s** into Eqs. 9 and 16, however, identified the results´ reliability in terms of accuracy.

4 Discussion

LCA has been developed for the assessment of environmental impacts of a product. To broaden the scope of LCA, Udo de Haes et al. (2004) propose three general strategies: the use of LCA in a toolbox, hybrid analysis, and the extension of LCA. Using LCA in a toolbox, the limitations shall be overcome by additional separate models that are used without a data link. The extension of LCA is considered with one consistent linear model. Thereby, LCA and the other tool are fully compatible. Hybrid modeling as a mixture of both approaches that combines LCA with other models and linking these by data flows. The extension with linear programming (LP) leads to a consistent linear model that determines the optimal choice among others for the total system under study. Interdependent choices in different regions can be studied simultaneously without matrix inversion, since with LP even rectangular systems can be solved. The criteria for choices are represented by the objective function (minimizing impacts on climate change) and the additional constraints (e.g., available feedstock in a region). It is shown that the modification of the program by additional profit requirements (LCC) into a goal program and a Pareto optimization approach also enables to incorporate multiple objectives within the decision-making process. Thereby, regional biomass availability and transport logistic options can be taken into consideration. The benefit of this

extension of LCA is to provide a broader and systematic assessment of consequences. The implicit environmental comparison of new bio-based technologies with fossil reference technologies can be regarded as a feature that has not been provided by other optimization models within the field of LCA. The LCC formulation used four our purpose is congruent to the suggestion of (Heijungs et al. 2013), since we only focus on the processes that provide the reference flows. However, it differs in the way that we only need to collect data for costs which are relevant for the decision-maker as a biorefinery investor and neglecting the costs for current technologies. This and the consideration of environmental targets can be interpreted as an eco-efficiency approach. However, instead of simply creating the fraction between an economic value and an environmental value (ISO 2012), the approach in this study allow to assess a specific target achievement, i.e. being less pollutant than current available technologies.

Dealing with multiple objectives, GP needs an a priori weighting of the different goals. In contrast, epsilon constraint method uses the concept of Pareto efficiency in which the solution is optimal in which an increase of a target would result in a decrease of another target. The advantage of GP is that one *optimal* solution can be determined whereas in the a posteriori method, the decision-maker is encouraged to decide for a compromise. Besides these two methods for multiple objective decision making, there exist further methods, which cannot be discussed here. A general overview including the pros and cons is given by Hwang and Masud (1979).

Rectangular LP models for choosing technologies have been used in input-output economics. Duchin and Levine (2011, 2012) introduced a rectangular model to study the

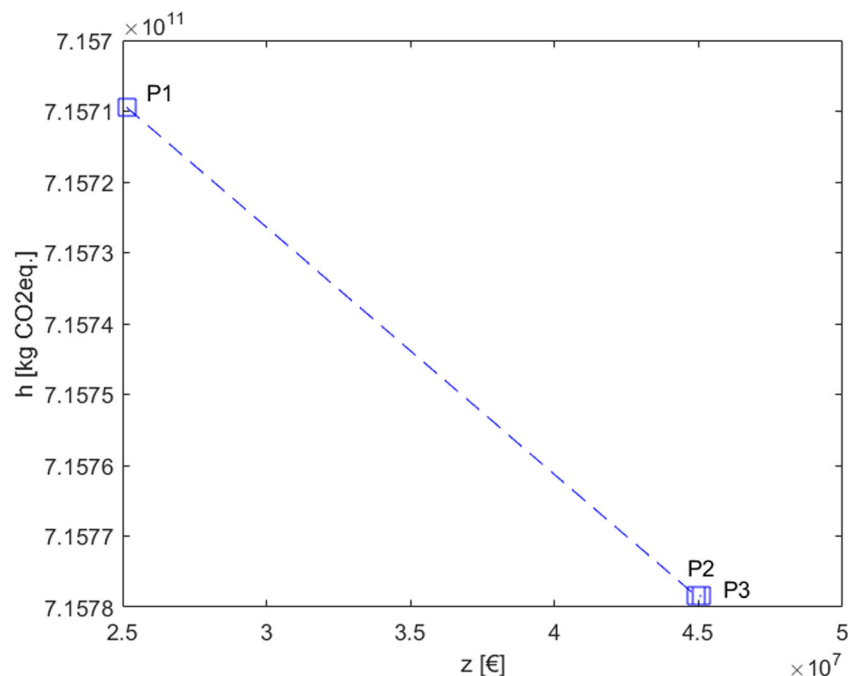**Fig. 5** Pareto front (50% scenario). h: environmental impacts; z: profit

Table 5 Results of the epsilon-constraint method (50% scenario), per annum

	P1	P2	P3
h (kg CO_2-eq.)	$7.15709438 \cdot 10^{11}$	$7.15778471 \cdot 10^{11}$	$7.15778469 \cdot 10^{11}$
z (€)	$2.514068 \cdot 10^{7}$	$4.492112 \cdot 10^{7}$	$4.509840 \cdot 10^{7}$
Biorefinery 1, Leuna (pc.)	1	0	0
Biorefinery 2, Leuna (pc.)	0	0	1
Biorefinery 1, Zeitz (pc.)	0	0	0
Biorefinery 2, Zeitz (pc.)	0	0	0
Biorefinery 1, Böhlen (pc.)	0	0	0
Biorefinery 2, Böhlen (pc.)	0	1	0
Biorefinery 1, Schwarzheide (pc.)	0	0	0
Biorefinery 2, Schwarzheide (pc.)	0	0	0

optimal choice of technologies. Before that, Carter (1970) applied a square choice-of-technology model using linear programming in a similar manner. Our model works in principle the same way. But instead of sectors as in input-output models, the columns of the technology matrix in LCA represent processes, which are usually modeled in more detail. Furthermore, these processes can be multi-functional (e.g., Kätelhön et al. 2016), which is contrary to input-output modeling in which the assumption of homogenous sector outputs is implied by creating the technical coefficient matrix (Miller and Blair 2009). In our example, only the biorefinery processes are multi-functional. Solving the multifunctional problem for these technologies can be interpreted as a system expansion approach. Furthermore, this approach is equivalent to substitution method, since the implicit aim of the introduced models is the substitution of current processes by less pollutant processes. To compare the biorefineries, the systems are expanded by current *substitutable* processes which produce the same type of products. Due to that a programming problem results, in which we seek to find the optimal substitution of current processes by a set of biorefinery alternatives. Other processes in the example are mono-functional. However, if other multioutput processes would be considered within the upstream processes of the biorefinery or the reference system, the multi-functionality can be solved by the program interpreting it as a kind of surplus method (Heijungs and Suh 2002). When minimizing the total environmental impacts of the system under study, larger amounts of supplied products would be allowed compared with those in the final demand. It is crucial to take this into consideration, since more products and hence more functions are possible in the final supply vector of the optimized system. On the other hand, if products of current technologies are not provided by the new technologies, the program would ensure that at least the amounts of the current system are generated. In this case a study would only be meaningful, if processes are modeled in a sufficient detailed manner. In other words, it must be decided which

process, e.g., a certain ethylene plant, is substitutable by the new process. Even in LCA, which uses more disaggregated processes than input-output analysis does, this is usually not the case. For instance, in our example only one process for ethylene generation represents a bundle of ethylene plants. Furthermore, the ethylene production is mono-functional, which does not represent real-life complexity, since ethylene usually is produced with other co-products (e.g., propylene). Including those co-products, however, can lead to binding constraints that are not achievable by the new technologies. In our example this becomes obvious if the *bundled* process of fossil ethylene production would additionally provide propylene. Since it seems not realistic to achieve a model that represents all production processes at a plant level, the only viable way is to make a model choice. The question is thus, what implicit assumption is appropriate in terms of the goal of the study (Zamagni et al. 2012). A general discussion is beyond the scope of this article. However, in terms of the predominant goal of the exemplary case studies, to identity the *best* alternative from a set of new biorefinery options, we argue that using aggregated mono-functional processes with average data seems to be sufficient. To increase the reliability of future case studies, however, the assessments should be enhanced by sensitivity analyses using different approaches for allocating the environmental impacts to the substitutable reference products (e.g., partitioning by physical and monetary factors).

Compared to common consequential LCA approaches which use substitution method to solve the multifunctional problem, the definition of determining products wherein all other co-products are summarized into one avoided product group (e.g., Weidema 2001; Suh et al. 2010) is not necessary. Here, in contrast, all products of the new technologies are considered as determining products without distinguishing between the multiple products. For each biorefinery product, substitutable reference products are determined. In our opinion, these choices for all products of the biorefineries seem closer to reality than whether clustering several co-products

into one avoided product group or declaring the multi-functional processes to be mono-functional by using partitioning method.

Towards a comprehensive LCSA framework, some potential directions for further research shall be broached. The characterization matrix $\mathbf{Q}$ can be easily modified by corresponding characterization factors to take into account additional environmental impact categories (e.g., midpoint or endpoint categories). Targets for various impact categories can be considered separately within a multi-objective framework. On the other hand, normalization and weighting could be introduced within a single environmental target function. Thus the optimization could be carried out in terms of a single environmental score which takes into account various normalized and weighted impact indicator results. In the same manner various social categories could be dealt with. By imposing a single score for each of the three pillars of sustainability (LCA, LCC, social LCA), the assessment of technological alternatives would be extended toward a comprehensive LCSA within a multi-objective framework. By identifying environmental, social, and economic benefits of new technologies (especially the comparison with existing technologies those produce equivalent products), this framework would be also suitable to support methods for estimating the maturity of technologies such as the technology readiness level (Hicks et al. 2009).

5 Conclusions

This article showed how (mixed integer) linear programming can be used to extend standard LCA towards comprehensive decision-making. Additional consequential research questions can be addressed such as the determination of the optimal number of new production plants and the optimal region for supplying feedstocks while also taking into consideration transport logistic options. The implicit environmental comparison of new bio-based technologies with fossil reference technologies can be regarded as a feature that has not been provided by other optimization models within the field of LCA. The extension of LCA by linear programming remains a consistent linear model, which is able to broaden the scope for consequential assessments. The benefit of this extension of LCA is to provide a broader and systematic assessment of consequences. The modifications of the program by additional profit requirements (LCC) into a goal program and Pareto optimization problem have been identified as promising ways toward a comprehensive multi-objective LCSA.

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