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Linking a farm model and a location optimization model for evaluating energetic and material straw valorization pathways—A case study in Baden-Wuerttemberg

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Abstract

Diminishing fossil carbon resources, global warming, and increasing material and energy needs urge for the rapid development of a bioeconomy. Biomass feedstock from agro-industrial value chains provides opportunities for energy and material production, potentially leading to competition with traditional food and feed production. Simulation and optimization models can support the evaluation of biomass value chains and identify bioeconomy development paths, potentials, opportunities, and risks. This study presents the linkage of a farm model (EFEM) and a techno-economic location optimization model (BIOLOCATE) for evaluating the straw-to-energy and the innovative straw-to-chemical value chains in the German federal state of Baden-Wuerttemberg taking into account the spatially distributed and price-sensitive nature of straw supply. The general results reveal the basic trade-off between economies of scale of the energy production plants and the biorefineries on the one hand and the feedstock supply costs on the other hand. The results of the farm model highlight the competition for land between traditional agricultural biomass utilization such as food and feed and innovative biomass-to-energy and biomass-to-chemical value chains. Additionally, farm-modeling scenarios illustrate the effect of farm specialization and regional differences on straw supply for biomass value chains as well as the effect of high straw prices on crop choices. The technological modeling results show that straw combustion could cover approximately 2% of Baden-Wuerttemberg's gross electricity consumption and approximately 35% of the district heating consumption. The lignocellulose biorefinery location and size are affected by the price sensitivity of the straw supply and are only profitable for high output prices of organosolv lignin. The location optimization results illustrate that economic and political framework conditions affect the regional distribution of biomass straw conversion plants, thus favoring decentralized value chain structures in contrast to technological economies of scale.

KEYWORDS

agricultural farm model, bioeconomy, bioenergy, biorefinery, lignocellulosic biomass value chain, location optimization, techno-economic analysis

1 | INTRODUCTION

The current global economic system depends strongly on finite resources. The world's population growth and the enlargement of the global middle class are likely to increase the demand for finite resources (Imbert, Ladu, Morone, & Quitzow, 2017). Likewise, apart from the quantitative limitation of raw materials in a fossil-based economy, the limitation of climate change requires the reductions of global CO_2 emissions (BP, 2018). In order to achieve the 2°C Global Temperature Target, a significant share of coal and gas reserves must remain unused (McGlade & Ekins, 2015). For this reason, policy-makers encourage the transformation of a fossil-based economy toward a bioeconomy. There are political strategies to promote the bioeconomy at European Union level (EC, 2012), at state (e.g., Germany) level (BMEL, 2014), and at federal state (e.g., Baden-Wuerttemberg) level (Hirth et al., 2013; WM, 2010). Within these strategies, the expansion of agricultural biomass use as a raw material is a crucial part in meeting the global challenges of climate change and the finite nature of fossil resources (IRENA, 2018). Simultaneously, an increased exploitation of agricultural biomass for energetic and material purposes competes with biomass for food and feed use and might consequently lead to an intensification of agricultural production causing negative environmental effects (Backhaus, Broers, Kögel-Knabner, Schwerin, & Thrän, 2015). For evaluation of these trade-offs, models can be applied to illustrate the economic and ecological impacts of future bioeconomy paths. In order to perform a prospective evaluation of the bioeconomy, a combination of multidisciplinary models from multiple sectors at different aggregation levels is necessary (Wicke et al., 2015). In addition to classical agricultural biomass such as grains or silage maize, lignocellulosic biomass will play an increasingly important role in the bioeconomy (Olsson & Saddler, 2013). As an important source of renewable energy, lignocellulosic biomass has been used for heat production ever since and lately serves as a resource for bioethanol production. In the future, lignocellulosic biomass such as agricultural and forestry residues might also replace fossil-based raw materials like crude oil and coal because of their valuable chemical compounds. Very promising products are biobased polymers such as lactic acid polymers or phenolic resins (Biddy, Scarlata, & Kinchin, 2016). In that regard, the EU has set new objectives to establish biorefinery operations for biofuels and chemical production by 2030 (BIC, 2017).

Whereas traditional bioenergy concepts generate electric and thermal energy by combusting lignocellulosic biomass, the innovative lignocellulose biorefinery concepts enable a full material utilization of the lignocellulosic components in order to obtain platform chemicals as a raw material for higher-value biomaterials. Thus, for biorefineries, the valuable component fraction within the feedstock is important, and for bioenergy plants, it is the energetic potential of the biomass. Despite these slightly different goals, the economic implementation of such concepts is characterized by a critical trade-off in planning biomass conversion plant locations. On the one hand, spatially scattered and fragmented availability of lignocellulosic biomass supply in combination with the relatively high water content and low energy density compared to fossil-based raw materials causes high transportation costs and affects the profitability of entire biomass value chains, esp. for bioenergy production (Giuntoli et al., 2013). On the other hand, technological economies of scale (EoS) call for larger conversion plants. The economic benefit is caused by the fact that the rate for machinery costs and other investments rises slower than the capacity of the plant (Remmers, 1995). Hence, centralized structures with large-capacity plants are more investment-efficient than decentralized plant structures, which aim to reduce transport distances and thus are more cost efficient in terms of transportation. In recent years, numerous publications have addressed this trade-off by different approaches. These publications can be distinguished, among other, by the breadth and depth of the evaluation of different production methods and processing stages of the value chain, as well as by the determination of the available feedstock supplies. Regarding the latter, many studies apply the technical or sustainable biomass potential while disregarding the economic constraints. In such studies, the biomass supply data are often taken from statistics. For instance, Ekman, Wallberg, Joelsson, and Börjesson (2013) estimate the feedstock supply based on official statistics and reports, and scientific literature. Ekşioğlu, Acharya, Leightley, and Arora (2009) calculate the biomass supply based on land availability and regionally differentiated yield levels. Marvin, Schmidt, and Daoutidis (2013) and Chen and Fan (2012) use official databases projecting regional differentiated prices and available quantities for individual feedstocks. Bussemaker, Day, Drage, and Cecelja (2017) consider limited variable forestry feedstocks with a predetermined fixed price. Rudi, Müller, Fröhling, and Schultmann (2017) formulate a mathematical model using existing potentials based on statistics in order to optimize the biomass value chain in terms of multiple feedstocks, technologies, and outputs.

Other studies adjust the statistical data by applying either a supply quota to ensure a sustainable utilization of biomass (Giarola, Zamboni, & Bezzo, 2011; Luo, van der Voet, & Huppes, 2010) or a predetermined share of arable land to produce feedstock (Lin, Rodríguez, Shastri, Hansen, & Ting, 2013). Zhang, Osmani, Awudu, and Gonela (2013) focus on biomass production on marginal land and derive biomass supply from the availability of marginal land. Other approaches determine the regional biomass supply based on agricultural production conditions on a high spatial resolution using geographic information systems (GIS) (Gonzales

& Searcy, 2017). Panichelli and Gnansounou (2008) apply a purely GIS-based approach to identify bioenergy locations in northern Spain. Parker et al. (2010) provide a consistent study of multiple conversion technologies competing for a diverse set of biomass feedstocks with real-world geographical data. Sukumara, Faulkner, Amundson, Badurdeen, and Seay (2014) use GIS to calculate a fixed maximum biomass supply for their location optimization. Wang, Liu, and Zhang (2013) combine a GIS-based statistical method with remote sensing to improve the spatial resolution and accuracy of the biomass supply for bioenergy. Tittmann, Parker, Hart, and Jenkins (2010) develop spatially explicit feedstock supply curves for various crop availabilities in their techno-economic approach. Wang, Hastings, and Smith (2012) derive feedstock supply by using a crop growth model for miscanthus. Other studies on biomass supply determination approach the topic from a monetary perspective. Sharma, Sarker, and Romagnoli (2011) present a financial planning model that maximizes stakeholder value based on land availability and yield level. Further studies emphasize the biomass storage (Ebadian, Sowlati, Sokhansanj, Townley-Smith, & Stumborg, 2013), the mode of transportation (Lin et al., 2016), or the impact of annual traffic growth rates (Bai, Hwang, Kang, & Ouyang, 2011).

Several studies perform a detailed analysis of agricultural biomass production for biorefineries. Egbendewe-Mondzozo, Swinton, Izaurralde, Manowitz, and Zhang (2011) identify profitable cropping systems by combining a terrestrial ecosystem model (EPIC) with a regional profit-maximizing mathematical programming model. Sokhansanj, Mani, Tagore, and Turhollow (2010) use detailed production and logistic options and weather conditions in order to estimate the biomass supply for biorefineries. Glithero, Wilson, and Ramsden (2013) conduct on-farm surveys and link them with farm accounting data to estimate straw supply for a potential bioethanol pathway. Other studies distinguish between different types of agricultural production. Thompson and Tyner (2014) estimate the costs of corn stover harvest and supply and then use that information to estimate farm production decisions and changes to farm profit at varying corn stover prices. Bai, Ouyang, and Pang (2012) present a game-theoretic model that incorporates farmers' decisions and market choices in the location optimization problem to integrate the competitive agricultural land use and the feedstock market equilibrium. Only few studies analyze the effects of an expanded bioeconomy with the help of farm models, which mainly apply mathematical programming. Louhichi et al. (2010) develop a bioeconomic farm model that can be applied in combination with models at high aggregation levels to assess policy questions under different biophysical and socioeconomic conditions. Banse et al. (2016) use a farm model within a model compound with a general equilibrium model and a partial equilibrium model for an analysis of

bioeconomy pathways, comprising agricultural, wood, and energy markets. According to our literature survey, not any study combines an agricultural farm model with a location optimization model to evaluate biomass value chains while integrating on-farm competition and technological EoS. For this reason, we propose the soft linkage of the agricultural farm model EFEM (Economic Farm Emission Model) (Kazenwadel, 1999) and the location optimization model Biomass value chain Integrated Optimization for LOcation, CApacity and TEchnology planning (BIOLOCATE) (Rudi, Müller et al., 2017) that considers spatially distributed and price-sensitive straw supply in a location optimization of biomass conversion plants.

Whereas EFEM applies regional agricultural production conditions and biomass prices and costs to estimate biomass supply, BIOLOCATE uses GIS-based input data (e.g., transport distances) in combination with techno-economic data (e.g., investments and capacities) to determine optimal biomass conversion plant locations. The linkage enables a transfer of data on biomass quantities and prices from the farm model to the location optimization model. The advantage of such model linkage consists in the consideration of the competitive situation of agricultural biomass supply and the most profitable locations of biomass conversion plants. Within this linkage, we also present a comparison of the classical biomass-to-energy pathway (BtE) and the innovative biomass-to-chemical pathway (BtC) while integrating price-sensitive agricultural production.

We focus on straw from wheat, barley (both spring and winter types), oat, and triticale as a by-product of grain cultivation. Straw offers the opportunity of a low competition between uses for either food and feed production (Weiser et al., 2014) and represents a highly unused potential in Baden-Wuerttemberg (Gauder, Graeff-Hönninger, & Claupein, 2011; WM, 2010). Although the energetic use of biomass comes along with possible ecological difficulties (e.g., flue gas cleaning), the energetic use of straw has a positive ecological performance (Tonini, Hamelin, & Astrup, 2016). In addition to the energetic use of straw, in the long term, a material use of biomass is inevitable in order to substitute fossil resources (Lewandowski, 2015). In this context, da Costa Sousa, Chundawat, Balan, and Dale (2009) and Anwar, Gulfraz, and Irshad (2014) identified the organosolv process as one of the most promising fractionation methods for lignocellulose biorefineries. The main advantage of organic solvents for pulping is the high purity of the obtained organosolv lignin, which allows easy processing into value-added products (Zhang, Pei, & Wang, 2016). Furthermore, C5 and C6 sugars can be fermented into platform and building block chemicals such as succinic acid, which is a promising precursor of many industrially important chemicals (Luo et al., 2010). Taking these aspects into consideration, we examine the established BtE pathway of straw combustion and the

innovative lignocellulose biorefinery concept as classified by the International Energy Agency Task 42 "Biorefining" for primary refining within the BtC pathway.

The main objective of the study was the application of a model linkage between a farm model and a location optimization model to the agro-industrial valorization of straw from herbaceous agricultural residues to evaluate the energetic and material valorization options from a regional perspective.

In the following sections, we introduce both models and their linkage as well present and discuss the integrated modeling results.

2 | MATERIALS AND METHODS

Agricultural biomass itself is relatively inexpensive, but has a low energy density. As a consequence, the economic profitability of such value chains critically depends on transportation costs. For this reason, logistics is of major importance when it comes to planning biobased value chains (Ba, Prins, & Prodhon, 2016). Additionally, on each farm, different farming productions compete for land. Therefore, the profitability of agricultural biomass production depends on different agricultural production conditions and specific farm capacities. Hence, it is fundamental to include provision, logistics, and conversion processes when evaluating biomass value chains. In this context, the provision process includes harvesting and pretreatment operations, and the logistics process includes storage, transport, and transshipment procedures.

2.1 | Biomass-to-energy (BtE) pathway

The BtE pathway is represented by the combustion of straw to generate heat and power within a capacity range of 3–25 MW_{el}. An average electric efficiency of $\eta^{el} = 0.0236 \cdot \ln(\chi^{el}) + 0.189$ and an average thermal efficiency of $\eta^{th} = -0.008 \cdot \ln(\chi^{el}) + 0.6457$ in accordance with the installed electric capacity χ^{el} are assumed (Rudi, Müller et al., 2017). The overall combustion efficiency is based on a 15% electric and a 60% thermal efficiency range as well as a scalable energy ratio resulting in a technology efficiency (η) of 25%. The large-capacity range enables an investigation of effects of Economies of Scale (EoS) and of governmental regulations on large-scale bioenergy systems such as the German Renewable Energy Act (REA). The considered bioenergy system integrates different types of combustion technologies such as the fixed- and fluidized-bed combustion in combination with steam turbines. Fixed-bed combustion is mainly applied in low-capacity ranges, whereas fluidized-bed combustion is more common in larger applications (Kaltschmitt, 2013).

As for all solid fuel combustion technologies, the boiler efficiency is related to the lower heating value (LHV) of the feedstock, which is assumed to be 14.2 MJ/kg for straw. The conversion process is modeled as a black box integrating the various subprocesses (e.g., on-site storage, pretreatment, combustion, and flue gas treatment), which is based on the scaling factor approach formulated by Rudi, Müller et al. (2017). The authors used research results from the project network entitled "Innovations for sustainable biomass utilization (OUI BIOMASSE)" to estimate the investment and the efficiency functions of the applied BtE pathway (Schumacher, Fichtner, & Schultmann, 2017).

2.2 | Biomass-to-chemicals (BtC) pathway

The integration of the BtC pathway is based on Engel, Fliedner, Fröhling, Haase, and Laure (2014) and the research network "Lignocellulose as new resource platform for novel materials and products" from the *Bioeconomy Research Program Baden-Wuerttemberg* (https://biooekonomie-bw.uni-hohenheim.de/en). The considered pilot-scale biorefinery concept utilizes straw to produces glucose (C6 sugars), high-purity lignin, and C5 sugars (in particular xylose) as output products by applying the organosolv pulping process. In contrast to conventional pulping processes (i.e., kraft, sulfite, or soda), the resulting organosolv lignin is characterized by little ash and carbohydrate impurities with a high Klason lignin content of approximately 90% and a molecular weight of 3,100 g/mol (Engel et al., 2014). The purity of lignin defines its application and the market price. High-purity lignin can be applied to substitute phenolic resins in binding agents or to synthesize polyurethanes in order to replace fossil-based products. Whereas the extracted glucose can be sold on the sugar market, the C5 sugar fraction is assumed to be a valuable raw material for the synthesis of xylitol and furfural, though its market potential is low in comparison with that of lignin and glucose (Mountraki, Koutsospyros, Mlayah, & Kokossis, 2017). The biochemical organosolv process converts lignocellulosic feedstock into its components with the highest fractionation rates by pulping with ethanol–water (Kleinert, 1974). Whereas cellulose is treated by enzymatic hydrolysis, lignin is precipitated from the mother liquor via water dilution and thermal precipitation. The organic solvent (i.e., ethanol) is recovered from the liquid process streams while the remaining C5 sugar fraction is extracted (Laure, Leschinsky, Fröhling, Schultmann, & Unkelbach, 2014).

In order to assess the energetic (BtE) and material (BtC) biomass valorization pathways for Baden-Wuerttemberg, we soft-link the agricultural farm model EFEM with the optimization model BIOLOCATE. Figure 1 shows the scheme of the developed model approach. By providing biomass supply volumes from EFEM and separating the supply costs, transport costs, and the technological profit in BIOLOCATE, an
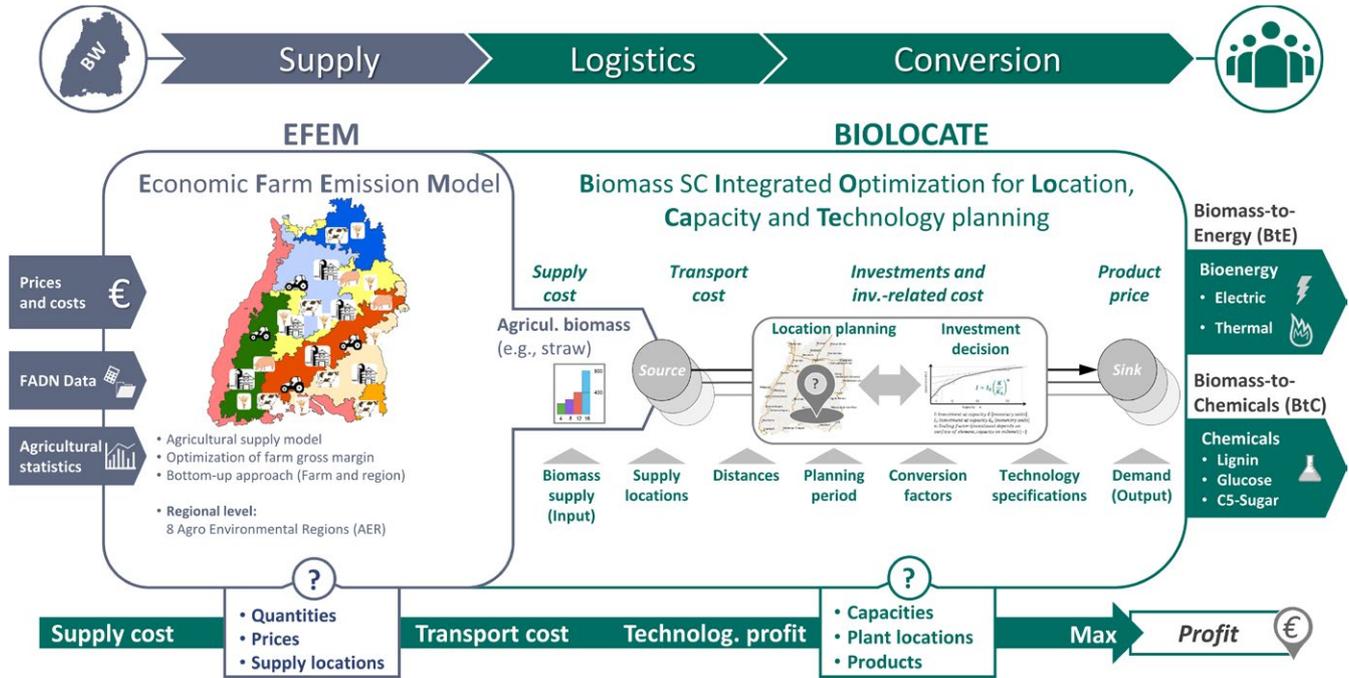
FIGURE 1 Scheme of model linkage

optimization of the value chain is performed by maximizing the overall profit of the system. The technological profit is defined as the revenue obtained by selling the output products subtracted by all occurring costs for producing the products excluding supply and transportation costs. These costs are integrated into the final location decision model.

2.3 | Agricultural production

The Economic Farm Emission Model (EFEM) is a comparative static linear optimization model, which maximizes the farms' gross margins. It operates in a bottom-up approach, which can be used at farm level as well as at regional level. Regionalization is achieved through extrapolation of the farm results. Figure 2 highlights the study area Baden-Wuerttemberg located in southwest Germany and shows the spatial resolution applied by EFEM. Baden-Wuerttemberg is divided into eight Agro-Ecological Regions (AER). These regions are characterized by similar agricultural production conditions, such as geological, topographical, and climate conditions (cf. Table 1). Although AER are on average five times as large as NUTS-3 regions (regional classification of the EU territory; cf. EC, 2016), they are more suitable for application in the study region. The different AER depict the regionally differentiated production conditions that result in different production foci. For example, there is a fertile crop farming region (AER 1), a region with less intensive forage farming in low mountain ranges (AER 3), and a region with intensive dairy production based on grassland (AER 5).
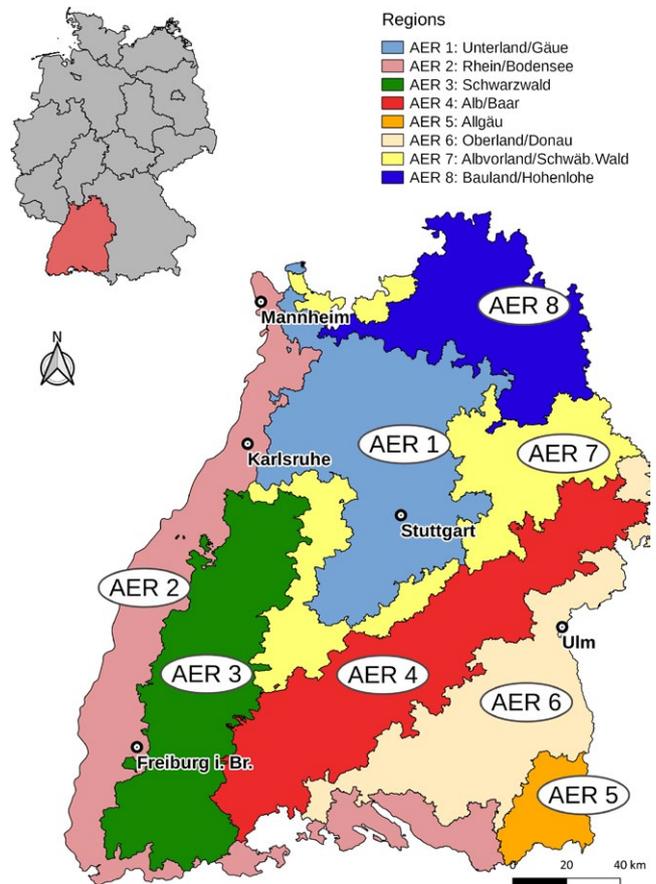

FIGURE 2 Study region (Baden-Wuerttemberg) in Germany and spatial resolution (AER) of EFEM

TABLE 1 Climate/agricultural characteristics of the Agro-Ecological regions (AER) in Baden-Wuerttemberg (LEL, 2018)

Agro-Ecological Regions	Unterland/Gäue	Rhein/Bodensee	Schwarzwald	Alb/Baar	Allgäu	Oberland/Donau	Albvorland/Schwäb. Wald	Bauland/Hohenlohe
	AER 1	AER 2	AER 3	AER 4	AER 5	AER 6	AER 7	AER 8
Elevation [m]	100–400	100–650	300–1000	600–1000	600–900	500–800	400–700	150–600
Avg. annual temperature [°C]	8.0–>9.0	8.0–9.0	5.5–>7.0	6.0–7.5	6.0–7.5	7.0–8.0	6.5–8.0	6.5–8.0
Avg. annual precipitation [mm]	650–750	550–1,100	800–1,500	600–1,100	1,000–1,600	650–800	700–1,000	600–1,000
Soil quality index (Ackerzahl) [0–100]	40–>80	20–70	20–40	20–40	30–50	30–60	20–60	30–50
Share of arable land [%]	65–100	30–80	20–50	30–55	<20	50–70	30–70	30–60
Agriculturally used area [ha]	241,095	190,862	105,072	220,459	47,862	244,935	177,128	182,575

The model consists of the farm type module, the production module, and the extrapolation module. The farm type module contains the different farm structures in each region. Each region is represented by a maximum of six typical farm models, for example, dairy farms or arable farms that depict the most common farm types in the individual region. Different sizes of a particular farm type per region are also possible. The general classification of these farm types is based on the farm typologies of the Farm Accountancy Data Network (FADN) (cf. EC, 2018b). The capacities of the typical farm models are based on average single farm data of the FADN and create restrictions for the optimization process. The main part of the model is the production module. It unites all relevant agricultural production operations of the plant and livestock production. EFEM distinguishes different production activities on arable land and grassland, which can be used as food or feed and in the BtE and BtC pathways. The different production processes can be varied in fertilization and plant production intensities.

Policy regulations and plant cultivation restrictions are also included in EFEM, for example, crop rotation, upper-limit usage of organic fertilizer, and equating of humus balance constraints. The latter is of particular importance for maintaining the soil fertility in production systems that remove organic matter from the fields, for example, by using straw rather than incorporating it into the soil (Cherubini & Ulgiati, 2010). The humus balance (HB) is calculated at farm level (r) and comprises the effect of different crops (D^{crop}) and manure (D^{manure}), as shown in Eq. 1. The effect of crops depends on the specific value per crop (k), yield level (w), and the use of the by-product (s). The effect of manure on humus is differentiated between pig and cattle manure. The balance at farm level depends on the specific production area for each crop (u) and the specific amount of manure (w).

$$\mathrm{HB}_r = \sum_{k \in F} u_{kr} \cdot D^{crop}_{kws} + \sum_{v \in M} w_{vr} \cdot D^{manure}_v \geq 0$$

With
$$F = \{\text{winter wheat, winter barley, } \cdots\}; \quad .$$
$$M = \{\text{pig manure, cattle manure}\}$$

(1)

In this context, the farms are able to cultivate intercrops to compensate the reduction of humus. Furthermore, the modeled farms are able to compensate the consequent nutrient removal through an adapted mineral and organic fertilization. All adaption strategies include their particular costs. The parameters of humus and fertilizer effects are based on VDLUFA (2014) and DüV (2017). The values of relevant input data, such as producer prices, factor prices, and yields, are based on 3-year averages to compensate the annual variability. The considered variable costs are exogenous parameters in the model that were obtained from official databases (cf. KTBL, 2017b; LEL, 2017a,b). The extrapolation module

projects the farm module results onto the regional level applying extrapolation factors. These factors are also defined by a linear optimization approach for depicting the entire agricultural production in each region. The agricultural census of 2010 provides the relevant regional capacities for the projection to AER level. Kazenwadel (1999) and Schäfer (2006) describe this modeling approach in detail, and a more recent application of EFEM can be found in Schwarz-v Raumer, Angenendt, Billen, and Jooß (2017) and Krimly, Angenendt, Bahrs, and Dabbert (2016).

Economic Farm Emission Model is calibrated to the base year 2010. The results of the model are validated against the agricultural census of 2010 by comparing data on animal numbers, crop production, and land use with statistical data. The comparison shows a difference in crop production of less than 10%, which is considered to be sufficient, and the complete area for fodder production is modeled 2% below statistics. The modeled livestock production shows a maximum deviation of 7% in comparison with statistical data of the agricultural census of 2010.

Logistic processes such as biomass collection, storage, and transportation are important cost drivers in biomass value chains. Concerning storage, we select square bales and on-field storage under tarps due to the cost advantages over other baling and storage types (Martelli, Bentini, & Monti, 2015; Sahoo & Mani, 2017). Contractors, paid by the farmers, perform the straw baling and collection to in-field stockyards. The straw price referred to in the following is the ex-field storage price, which includes the baling and storage costs expressed in euros per ton of fresh matter ($€/t_{FM}$). The straw quantity is expressed in fresh matter with a dry mass content of 86%. Further logistic processes including the un-/loading and transportation are implemented in the BIOLOCATE model.

2.4 | Location planning (BIOLOCATE)

Different biomass valorization pathways exist, starting from the provision of biomass feedstock through to the logistics, and the conversion of biomass. Each pathway consists of interactive planning tasks and multiple decisions, such as the type and source of biomass feedstock, the quantity to be transported, and the conversion technology to be chosen in order to produce a certain output product (Schwaderer, 2012). Considering the multiplicity of conversion technologies and products, as well as biomass price elasticities, the use of linear models is highly recommended, as they are easy to apply, reduce computation time, and ensure optimality (De Meyer, Cattrysse, Rasinmäki, & van Orshoven, 2014; Hong, How, & Lam, 2016). The BIOLOCATE model is a mixed integer linear programming model (MILP), which models strategic decisions within biomass value chains. Such decisions concern the location planning of biomass conversion plants while

taking into account technological EoS. EoS are generally larger for centralized large-scale conversion plants than for multiple smaller and decentralized ones because the former need less specific investments while increasing the geographic catchment area of biomass feedstock. However, unlike fossil resources, biomass feedstock, due to low energy density, favors a cost-effective short-distance transportation, resulting in a decentralized network structure with small- or medium-scale conversion plants (Fiedler, Lange, & Schultze, 2007; Kaltschmitt, Hartmann, & Hofbauer, 2009; Kudakasseril Kurian, Raveendran Nair, Hussain, & Vijaya Raghavan, 2013; Wiese, 2013; Yue, You, & Snyder, 2014). The integration of this trade-off assumption between EoS and transportation costs requires advanced modeling techniques to assess biomass valorization pathways while incorporating various types of biomass feedstock, the multiplicity of conversion processes, and many output products (Fröhling, Schweinle, Meyer, & Schultmann, 2011; Sharma, Ingalls, Jones, & Khanchi, 2013). Numerous models analyze biomass valorization pathways (Ba et al., 2016; Garcia & You, 2015; Yadav & Yadav, 2016), but disregard the trade-off assumption (Batidzirai, 2013; Shastri, Rodriguez, Hansen, & Ting, 2012) and the price elasticity of the biomass feedstock (Panichelli & Gnansounou, 2008). The presented model integrates the price elasticity of agricultural biomass feedstock and enables location planning of biomass conversion plants based on a techno-economic analysis (TEA) of biomass-to-energy (BtE) and biomass-to-chemical (BtC) pathways. The TEA integrates different capacity ranges of conversion technologies in comparison with the associated investments (Ekşioğlu et al., 2009; Zhang, Johnson et al., 2016). Important factors of the TEA are the capital and operational expenditures for building conversion plants, such as biomass power plants (BtE) and biorefineries (BtC).

An economic evaluation of biomass value chains is provided while integrating relevant cost and investment factors in accordance with the German VDI 6025/2067 guidelines (VDI, 2012a,b). These factors comprise the gross investment, the income from current operations, as well as capital and operational expenditures, and are uniformly discounted over the planning period of 20 years in accordance with the annuity method. The expenditures consist of the costs of feedstock and fuel, maintenance and repair, as well as insurances, taxes, and costs of labor, utilities, operating material, supplies, administration and overhead, and the disposal of residues and ash (Eltrop, 2014).

The main characteristics of the model are described by relevant model equations, whereas the model notation is summarized in Table 2. Both the energetic and the material valorization pathways are integrated into one model formulation to compare the straw valorization for bioenergy generation and production of chemical components, that is, lignin, glucose, and C5 sugars. The starting point of the value chain

TABLE 2 Indices, variables, parameters, and equations of BIOLOCATE

Indices	
$b \in \{1, \dots, B\}$	Type of biomass feedstock
$i \in \{1, \dots, I\}$	Biomass supply location (source)
$j \in \{1, \dots, J\}$	Conversion plant location (sink)
$p \in \{1, \dots, P^{BtE}, P^{BtC}, P\}$	Conversion technology
Variables	
$x_{bijp} \in \mathbb{R}^+$	Continuous variable: biomass flow [t_{FM}/year]; $\forall b \in \{1, \dots, B\}, i \in \{1, \dots, I\}, j \in \{1, \dots, J\}, p \in \{1, \dots, P\}$
$y_{bjp} \in \mathbb{N}_0$	Integer variable: number of installed plants per location; $\forall b \in \{1, \dots, B\}, j \in \{1, \dots, J\}, p \in \{1, \dots, P\}$
Z	Objective function value of profit to be maximized [€/year]
G^{Profit}	Profit of the complete biomass value chain [€/year]
$C^{Biomass}$	Costs of biomass feedstock [€/year]
$C^{Transport}$	Costs of biomass transport [€/year]
$p^{el}(\tau_p, \chi_p^{el})$	Price of electrical energy depending on the plant availability and installed capacity [€/kWh$_{el}$]
$\omega^{th}(\chi_p^{th})$	Relative share of sold thermal energy depending on installed capacity of BtE conversion technology
Parameters	
a_{bi}	Supply quantity of biomass feedstock b at source location i: [t_{FM}/year]
I_p	Investments for BtE conversion technology p: [€/year]
I_p^{CAPEX}, I_p^{OPEX}	Basis value of the expenditure function of BtC conversion technology p: [€], [€/t], [€/kWh]
$c_b^{Biomass}$	Supply costs of biomass feedstock b: [€/t_{FM}]
c_b^{fixT}	Fixed transportation costs of biomass feedstock b: [€/t_{FM}]
c_b^{varT}	Variable transportation costs of biomass feedstock b: [€/(t_{FM}km)]
d_{ij}	Road distance between biomass source location i and conversion plant location j: [km]
f_{pb}	Demanded quantity of biomass feedstock b for conversion by technology p: [t_{FM}/year]
g_p^{BtE}, g_p^{BtC}	Investment profit of technology p for BtE and BtC conversion: [€/year]
lhv_b	Lower heating value of biomass feedstock b: [MJ/t_{FM}]
n_p^{CAPEX}, n_p^{OPEX}	EoS scaling factor for capital (0.7) and operational expenditures (0.95) of BtC conversion technology p: [-]
o^{th}	Relative loss of thermal energy in the district heat network: [%]
p_p^x	Price of output product x (i.e., lignin, C5 sugars, C6 sugars) produced by BtC conversion technology p: [€/t_{FM}]
p^{th}	Price of thermal energy generated by BtE conversion: [€/kWh$_{th}$]
q^{th}	Costs of expanding the district heating network: [€/kWh$_{th}$]
β_p, β_p^0	Basis capacity and actual capacity of BtC conversion technology p: [t_{FM}/year]
$\beta_p^{min}, \beta_p^{max}$	Lower/upper limit for installed electrical power of BtE conversion technology p: [MW$_{el}$]
η_p^{el}	Electrical efficiency of BtE conversion technology p: [%]
η_p^{th}	Thermal efficiency of BtE conversion technology p: [%]
τ_p	Operation time of conversion technology p: [hr/year]
χ_p^{el}, χ_p^{th}	Installed electrical/thermal capacity of BtE conversion technology p: [MW$_{el}$], [MW$_{th}$]
ϑ_{bp}^x	Factor for converting biomass b into output x (i.e., lignin, C5 sugars, C6 sugars) through BtC technology p: [-]
Equations	
Objective function	$\max Z = G^{Profit} - C^{Biomass} - C^{Transport}$ (2)
System profit	$G^{Profit} = \sum_{b=1}^{B} \sum_{j=1}^{J} \sum_{p=1}^{P} g_p \cdot y_{bjp}$ (3)
Biomass supply costs	$C^{Biomass} = \sum_{b=1}^{B} \sum_{i=1}^{I} \sum_{j=1}^{J} \sum_{p=1}^{P} c_b^{Biomass} \cdot x_{bijp}$ (4)
Transport costs	$C^{Transport} = \sum_{b=1}^{B} \sum_{i=1}^{I} \sum_{j=1}^{J} \left(\left(c_b^{fixT} + c_b^{varT} \cdot d_{ij} \right) \cdot \sum_{p=1}^{P} x_{bijp} \right)$ (5)

(Continues)

TABLE 2 Continued

Equations			
Supply of biomass	$\sum_{j=1}^{J}\sum_{p=1}^{P} x_{bijp} \le a_{bi}$	$\forall b \in \{1,\ldots,B\} \forall i \in \{1,\ldots,I\}$	(6)
Process supply at conversion plant	$\sum_{i=1}^{I} x_{bijp} = f_{bp} \cdot y_{bjp}$	$\forall b \in \{1,\ldots,B\} \forall j \in \{1,\ldots,J\}$ $\forall p \in \{1,\ldots,P\}$	(7)
Input of biomass for BtE conversion	$f_{bp} = \dfrac{\chi_p^{el}\cdot\tau_p\cdot 3,600\frac{s}{hr}}{lhv_b\cdot\eta_p^{el}}$	$\forall b \in \{1,\ldots,B\}\ \forall p \in \{1,\ldots,P^{BtE}\}$	(8)
BtE conversion and capacity constraint	$\chi_p^{th} = \dfrac{\chi_p^{el}}{\eta_p^{el}}\cdot\eta_p^{th}; \beta_p^{min} \le \chi_p^{el} \le \beta_p^{max}$	$\forall p \in \{1,\ldots,P^{BtE}\}$	(9)
Investment profit of BtE conversion	$g_p^{BtE} = (10 \cdot p^{el}\left(\tau_p, \chi_p^{el}\right)\cdot\chi_p^{el} + 10\cdot(p^{th}-q^{th})\cdot(1-o^{th})\cdot\omega^{th}\left(\chi_p^{th}\right)\cdot\chi_p^{th})\cdot\tau_p - I_p$	$\forall p \in \{1,\ldots,P^{BtE}\}$	(10)
Investment profit of BtC conversion	$g_p^{BtC} = p_p^{x}\cdot\vartheta_{bp}^{x}\cdot f_{bp} - \left(I_p^{CAPEX}\left(\dfrac{\beta_p}{\beta_p^0}\right)^{n^{CAPEX}} + I_p^{OPEX}\cdot\left(\dfrac{\beta_p}{\beta_p^0}\right)^{n^{OPEX}}\right)$	$\forall b \in \{1,\ldots,B\}\ \forall p \in \{1,\ldots,P^{BtC}\}$	(11)

is the biomass source location *i*, for example, an agricultural farm, which provides a type of feedstock *b*, for example, straw. The quantity of feedstock supply is price-sensitive for every source location. Biomass is transported to a sink location *j* in order to be converted with technology *p*. Conversion technologies are modeled in their entirety; hence, individual processing and conditioning activities at different locations as well as pretreatment measures and intermediate products are not modeled separately in contrast to other modeling approaches developed by, for example, De Meyer, Cattrysse, and van Orshoven (2015, 2016).

The MILP formulation maximizes the profit of BtE and BtC pathways (2), cf. equations in Table 2. It consists of the revenue of selling output products, such as bioenergy or chemical components (3), subtracted by occurring costs and investments for a planning period of 20 years. Bioenergy in the form of heat and power is generated through combustion. The installed electric power corresponds to the output product, which is fed into the power and district heat network and then sold (10).

Whereas bioenergy is generated by burning straw, chemical components are produced through the primary refining step by applying the organosolv process. The particular lignocellulose biorefinery concept is implemented as a top-down approach according to the German VDI 6310 guideline (VDI, 2016). In accordance with the biomass input flow, conversion factors transform the lignocellulosic feedstock into its components while capital and operational expenditures are taken into account to estimate the costs (11). The total expenditures are broken down into biomass feedstock costs (4), provided by EFEM; transport costs (5), corresponding to average logistics service provider rates; investments, and auxiliary costs, estimated by the application of scaling factors.

Whereas Eq. (4) in Table 2 represents the sum of biomass supply costs for the selected LAU 2 source regions taking into account different price-to-quantity ratios, Eq. (5) in Table 2 considers the fixed and distance-dependent road transport

costs offset with the biomass volumes to be transported from the source to the specific sink locations.

The system boundaries are defined by the source and sink locations that are located in the federal state of Baden-Wuerttemberg. However, the BIOLOCATE model can be applied to any other geographical region. The flow of biomass feedstock is represented by a continuous variable ($x_{bijp} \in \mathbb{R}^+$), and the decision on the location is represented by an integer variable ($y_{bjp} \in \mathbb{N}_0$). Whereas x_{bijp} defines feedstock-dependent costs and restrictions, the location decision variable y_{bjp} represents the number of installed plants per location, enabling the allocation of investments and auxiliary costs to specific locations.

Although biomass is spatially distributed, we assume that the price-sensitive biomass feedstock is supplied at 1,104 source locations (6), which represent the second level of local administrative unit (LAU 2) municipalities of Baden-Wuerttemberg. The volume of biomass x_{bijp} is variable and cannot exceed the parameter a_{bi}, which is the volume of biomass supply at one LAU 2 region (*i*). It depends on the price that is offered at that specific LAU 2 region. LAU 2 is the building blocks of the European NUTS regions; they comprise the municipalities and communities of the European Union, which for Baden-Wuerttemberg range from 100 ha to 44,000 ha (EC, 2016). The centroid of these LAU 2 locations is assigned to 40 candidate sink locations forming a road transportation network without any storage or transshipment activity. Potential biomass conversion plant locations in Baden-Wuerttemberg have been investigated by Schwaderer (2012) in accordance with certain criteria as shown in Figure 3. At first, the distance to settlement areas, the topography, and the land use, for instance, define spatial criteria in order to determine candidate plant locations in the geographical boundaries of Baden-Wuerttemberg (analysis of potential plant locations). By linking the source and sink locations of the biomass flow with the road network, the transport distances are calculated in the second step (transportation

network definition). The final layer used in the BIOLOCATE model consists of a set of distance doublets (source: i, sink: j).

If a conversion plant operates with a certain capacity, the required feedstock input is ensured (7) assuming an operation period for combustion plants of 7,000 and for biorefineries of 8,000 full-load hours per year (Haase, 2012; Zeller et al., 2012).

The implemented combined heat and power (CHP) technology produces electric and thermal energy simultaneously via the conversion process of combustion (8). The generated bioenergy is calculated based on the technical efficiencies, the feedstock availability, and implicit input variables, such as the water content of the feedstock (9). For an operational time frame of 20 years, the price of electric energy is conditioned by the rated power of the plant and calculated in accordance with the subsidy amount from remunerations under the German Renewable Energy Act (REA, 2014) for the production year 2015. While the electrical energy is entirely distributed, thermal energy is sold at a reasonable price of 0.06 €/kWh$_{th}$ (AGFW, 2017), taking into account the grid extension costs and heat losses by assuming an existing heat demand (10).

In addition to the price-dependent biomass supply, the final investment decision depends largely on the capacity of the conversion plant. As proposed by Koch (2009) and Schatka (2011), the presented modeling approach applies 25 individual discrete values of the capacity curve for investment estimations. These include an investment cost factor of 0.17 for auxiliary costs such as tax, operation and maintenance, and labor costs in accordance with Schwaderer (2012). Depending on the scale-up factors, a set number of scale-up capacities for the combustion and chemical conversion of

straw into chemical components are used to formulate the mathematical problem (10 and 11). The profit estimation of the biorefinery concept results from the revenue obtained from selling the converted chemical components minus the capital and operational expenditures. The capital expenditures comprise plant equipment such as compressors, heaters, and coolers for solvent recovery, reactors for decomposing lignocellulosic biomass, equipment for lignin and cellulose washing as well as lignin precipitation, reactors for hydrolysis, and devices for lignin separation. The operational expenditures include costs of fossil-based ethanol (500 €/$t_{Ethanol}$), enzymes (36 €/$t_{Glucose}$), process water (0.15 €/$t_{Feedstock}$), power (0.11 €/kWh), and heat (24-28 €/$t_{Feedstock}$). Some heat is generated from burning the hydrolysis lignin, the remaining heat is generated from heaters. Electricity for running the biorefinery is supplied from the grid. Hence, the considered biorefinery is not energy self-sufficient, which at the current state of technology development is a realistic assumption (Wertz & Bédué, 2013).

The MILP model integrates strategic decisions on location, capacity, and technology planning in order to provide a techno-economic analysis of biomass value chains. Such decisions cover the straw quantity to be supplied, transported, and converted to either bioenergy or chemical raw materials at various plant locations with different capacities in order to maximize the profit of the value chain. The model is applied to the agro-industrial valorization of straw from herbaceous agricultural residues to evaluate the energetic and material valorization options from a regional perspective. The input data covers the economic biomass potential of spatially distributed price-sensitive quantities of straw from EFEM.
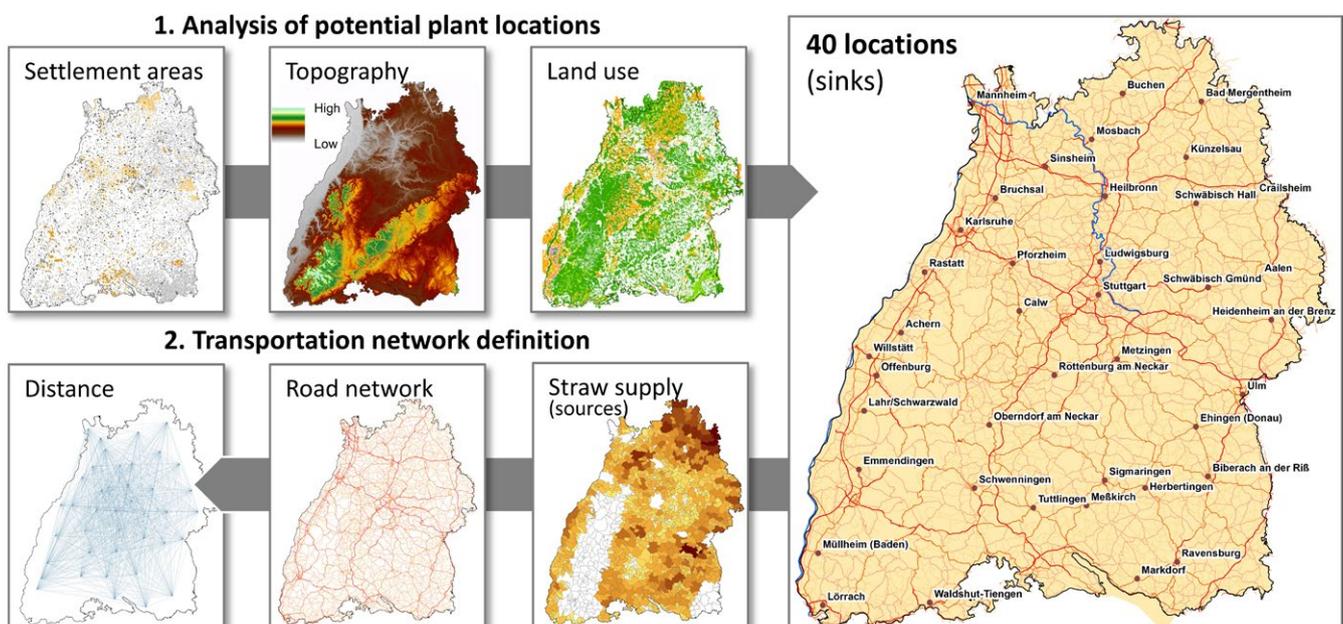

FIGURE 3 Criteria for the selection of potential biomass conversion plant locations (1) and determination of transportation network (2)

2.5 | Model linkage

BIOLOCATE requires feedstock supplies at a LAU 2 level. However, the biomass production output of EFEM is at the regional level of AER. Accordingly, the modeled biomass supply of EFEM has to be spatially distributed to the LAU 2 level in order to process the location optimization with BIOLOCATE. In this approach, we assume that the modeled crop rotation in the AER is the same in each LAU 2 region. The administrative LAU 2 regions are assigned to the respective AER and are determined by a two-step distribution. First, the overall straw production per AER is converted into an average yield per hectare using the available amount of arable land. Then, the straw yield of that particular crop rotation in the individual AER is assigned to each LAU 2 region and then multiplied by the respective arable land area. This quantity at LAU 2 level is subsequently transferred to BIOLOCATE. The statistics of arable land at LAU 2 level and of the AER in this spatial distribution are based on the Agricultural Census 2010 (DESTATIS, 2010).

Besides the integrated animal husbandry production systems, a few production systems are not considered in EFEM. Horse husbandry is not implemented because horse owners' high willingness to pay makes farm-level implementation in economic linear optimization approaches difficult. Furthermore, sheep farming only plays a minor role in Baden-Wuerttemberg, and for this reason, it is not included in EFEM. In order to take this into account, we extrapolate the straw demand for the not integrated animal bedding and feed based on animal numbers and average straw demands in accordance with Rösemann, Haenel, and Dämmgen (2015) and KTBL (2017a). These demand volumes are deducted from the modeled straw supply and are therefore not available for conversion.

3 | RESULTS

3.1 | Straw supply

In order to depict straw supply with different prices, we run EFEM with eleven scenarios. Each scenario reveals the straw supply at a particular price. In addition to the baseline scenario, we model the straw supply between 30 and 80 €/t_{FM} ex field in steps of 5 €/t_{FM}. Figure 4 shows the corresponding straw supply curves for each AER. The straw supply increases in each region with increasing price. This is caused by different marginal costs of straw supply of the farms, which are based on different agricultural production conditions and farms' specific costs to compensate the removal of nutrients and humus. The shape of the supply curves shows differences between the regions. In most regions, the supply curve shows a relatively constant supply for up to a price of 40 €/t_{FM} and a strongly increasing progression between 50 and 60 €/t_{FM}. This range represents the best price-to-quantity ratio of straw supply. AER 1, AER 6, and AER 8 provide approximately 500 kt_{FM} at most, and the supply curves are characterized by a high progression at a straw price of 50 €/t_{FM}. These regions have a high number of cropping farms and area of arable land. Hence, the competition between the use of straw for innovative BtE and BtC valorizations and traditional agricultural use such as feed is less pronounced. This
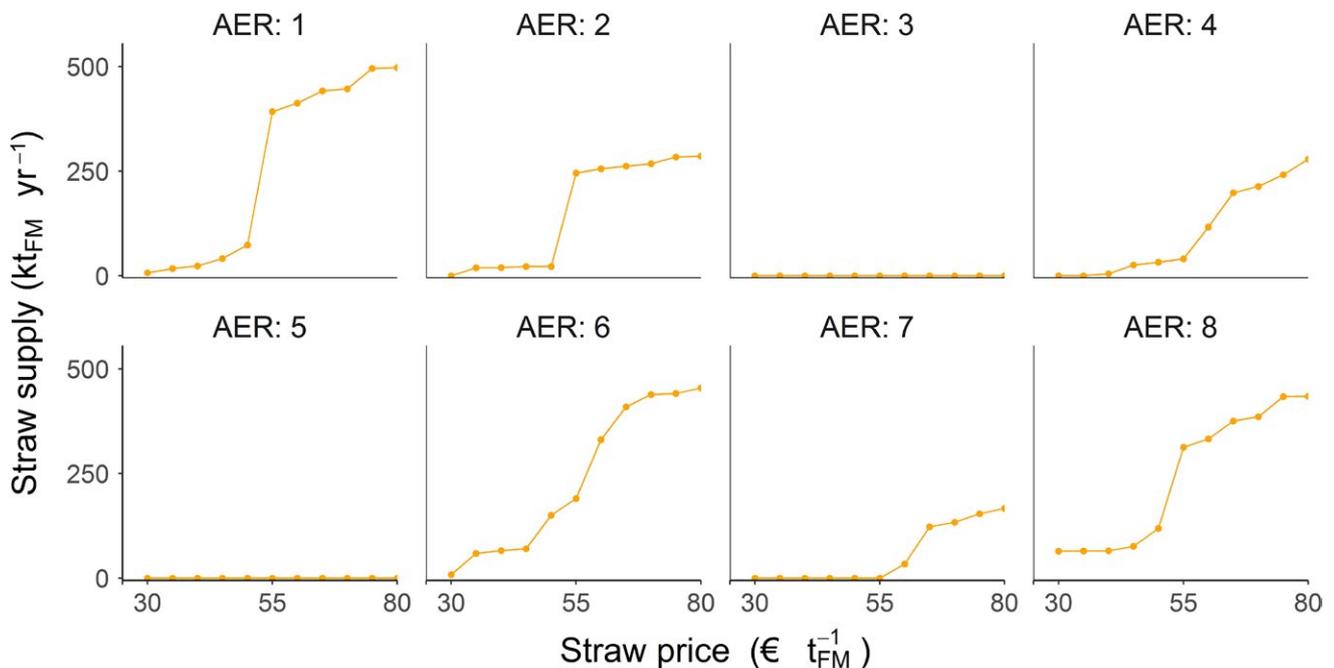

FIGURE 4 Modeled straw supply curves per AER

results in a relatively high straw supply in these regions. The modeled maximum straw supply for AER 2 and AER 4 is approximately 300 kt_{FM} for a straw price of 80 $€/t_{FM}$. In AER 2, the straw production has to compete with a pronounced corn production. This corn production is relatively profitable and limits the use of straw to the already cultivated cereals in the crop rotation. This is the reason for the flat run of the straw supply curve at straw prices above 80 $€/t_{FM}$ compared to the other regions. In AER 7, the maximum straw supply amounts to around 170 kt_{FM}. In AER 3 and AER 5, even for a price of 80 $€/t_{FM}$, no straw supply is available. The latter two regions are characterized by a strong competition for arable land between cattle and dairy farming and cash crop production. Due to the higher profitability of cattle and dairy farming per area, the arable land is mainly used for growing forage (silage maize and grass-clover), and relatively small amounts of grain.

3.2 | BtE location optimization

The BIOLOCATE model optimizes for the most profitable combination of biomass supply while taking into account, the specific biomass prices at each source location in order to produce a certain amount of energy at specific locations. Figure 5a shows the results of straw combustion plant location planning in Baden-Wuerttemberg. Whereas connecting

lines illustrate the feedstock flow from LAU 2 regions to the combustion plants, different color schemes represent the consumed quantities of feedstock. The feedstock prices ranging between 50 and 60 $€/t_{FM}$ with an average of 55 $€/t_{FM}$ are additionally highlighted. The average road transport distance from the source locations of straw supply to the combustion plants is 23 km, whereas the longest distance is 91 km.

The total system profit accounts for approximately 30 million €/year, which is generated at 34 of the 40 candidate plants with an overall installed electric capacity of 213.65 MW and a thermal capacity of 563 MW. Of these plants, 33 have an installed capacity of 6.3 MW_{el} and one of 5.75 MW_{el} (cf. green squares in Figure 6). One location contains three plants, and four locations contain two plants. The remaining locations consist of one plant. The plants convert a total of 1,538 kt_{FM}/year of straw to produce 1.49 TWh of electricity, which corresponds to 2% of the gross electricity consumption and 3.94 TWh of thermal energy that correspond to 35% of the district heating consumption of Baden-Wuerttemberg (Stala BW, 2018). In the case of district heating, however, it should be noted that only a small proportion of the households (7%) are supplied with districted heating. The total costs consist of a 10% share of technology investments, 25% share of transportation costs, and 65% share of straw supply costs.
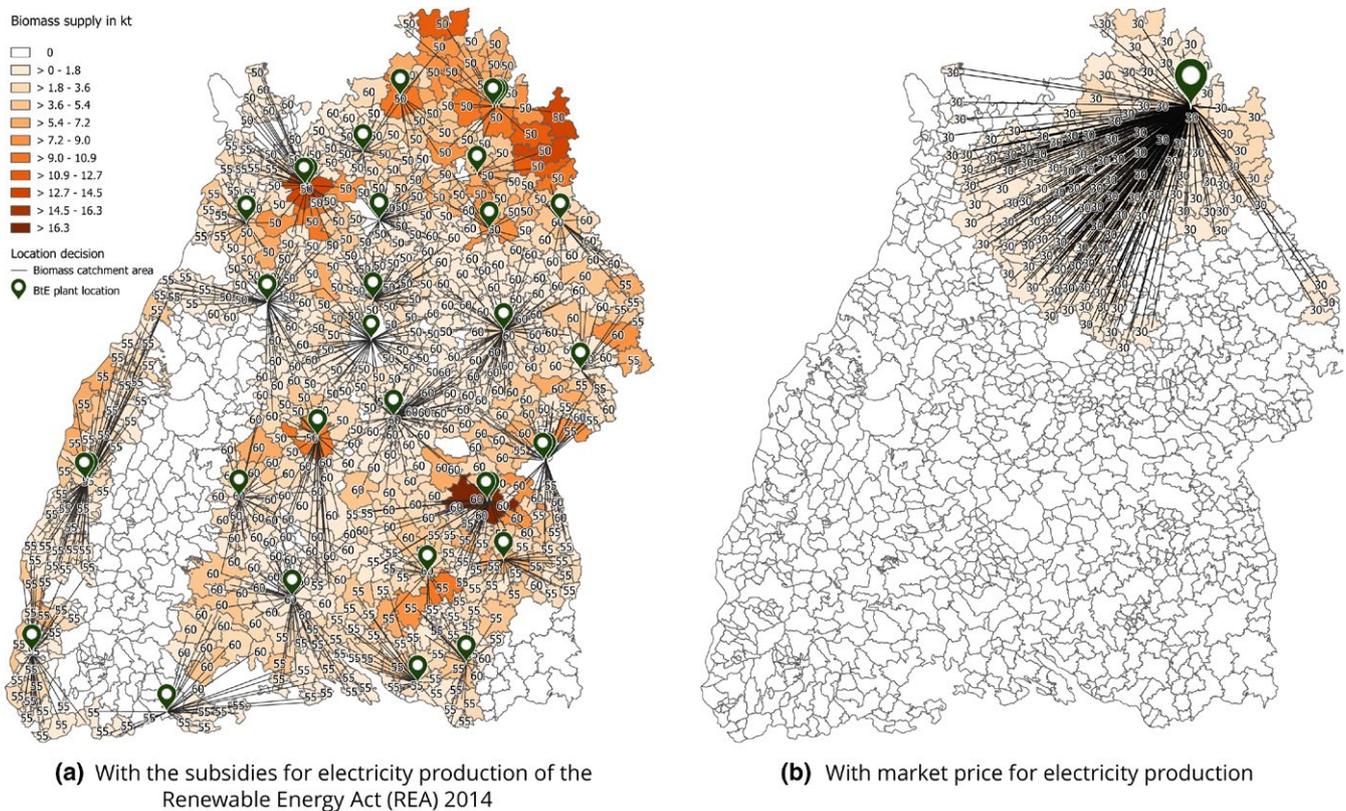

(a) With the subsidies for electricity production of the Renewable Energy Act (REA) 2014

(b) With market price for electricity production

FIGURE 5 Modeling results of combustion plant location planning and priced straw supply flows at LAU 2 level
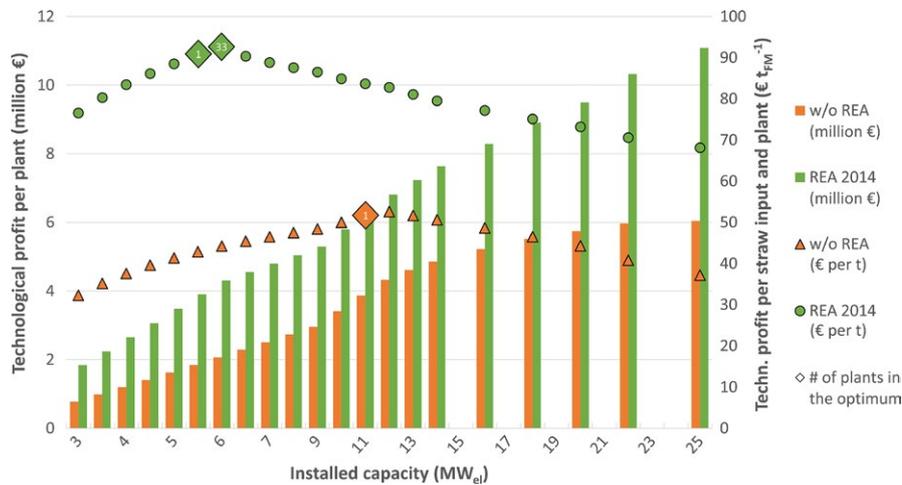
FIGURE 6 Technological profit per plant of applying combustion technology per straw input without transportation and supply costs with and without (w/o) the feed-in tariff of the Renewable Energy Act (REA, 2014)

The optimal BtE location decisions are influenced by the feed-in tariff of the German Renewable Energy Act (REA, 2014). The feed-in tariff provides a surcharge to the energy price in order to help finance biomass combustion technologies. Its consideration results in a decentralized plant allocation of low-capacity combustion plants. In accordance with this regulation, a feed-in tariff up to a rated capacity of 5 MW_{el} and corresponding to an installed capacity of 6.3 MW_{el} is economically favorable. Such plants are the most profitable ones under the considered model assumptions due to the highest ratio between technological profit and input quantities, as shown in Figure 6. In addition, Figure 6 shows a scenario without the REA feed-in tariff. Whereas the green dots and the orange triangles represent the ratio in €/t_{FM} per plant between the technological profit and the input straw volumes, the green and orange pillars highlight the absolute technological profit in million € per plant with a nonlinearly increasing installed capacity. Assuming a market price of electric energy of 0.03 €/kWh_{el} (EEX, 2017) and of thermal energy of 0.1 €/kWh_{th}, a scenario without the REA feed-in tariff is defined. Although a realistic price of thermal energy is 0.06 €/kWh_{th}, only prices above 0.1 €/kWh_{th} enable profitable solutions for the location optimization. In contrast to the feed-in tariff scenario, which benefits plant capacities of up to 5 MW_{el}, the market price scenario without the feed-in tariff favors high-capacity combustion plants in a range of 9–12 MW_{el}. However, the economic benefits are much lower due to the missing surcharge, as shown by the comparison of the two dotted lines. Therefore, only one plant with a capacity of 10.7 MW_{el} is implemented (as indicated in Figure 6 by the orange squares) in the northeastern part of Baden-Wuerttemberg (Figure 5b). Despite a low straw price of 30 €/t_{FM}, the plant barely reaches the break-even with a total profit of 10,142 € per year. The concavity of the two continuous lines is explained by the application of different CHP technologies, for example, fixed-bed firing,

fluidized-bed combustion, and the assumed average technology efficiency. The updated version of the REA 2017 does not provide significant changes in the feed-in tariff in comparison with the REA 2014. Hence, we only expect a slight decrease in the technological profit, but no major effects on the modeling results.

3.3 | BtC location optimization

Similar to the BtE location optimization, the optimal BtC location decision is influenced by the classical trade-off between EoS and transportation costs. Hence, one would expect a highest capacity biorefinery in the center of the transportation network to be optimal; however, the capacity decision is significantly affected by the straw supply price as well. In order to understand the choice of the optimal biorefinery location and capacity, four restricted plant capacity scenarios are modeled. The scenario results are presented in Figure 7 and show the optimal locations in size proportion for a plant capacity size of 0.5 (Figure 7a), 1.0 (Figure 7b), 1.1–1.7 (Figure 7c), and 1.8-2 (Figure 7d) million t_{FM} of straw per year. Each of these four capacity scales results in different optimal biorefinery locations. Out of these capacity scales, the overall optimal capacity is 1.6 million t_{FM}, although the maximum straw supply quantity at a price of 80 €/t_{FM} is 2.1 million t_{FM} (cf. Figure 4).

Unlike the results of the BtE pathway, only one optimal candidate location for a biorefinery has been selected near Stuttgart (cf. Figure 7c). The high-capacity biorefinery consumes a total of 200 t_{FM}/hr, which corresponds to an annual straw demand of 1,600 kt_{FM}. The selected straw price varies between 50 and 70 €/t_{FM} with an average price of 56 €/t_{FM}. The majority of the LAU 2 regions (85%) provide straw at a price of either 55 or 60 €/t_{FM}. The consumed feedstock supply ranges between 0.12 and 18 kt_{FM} of straw for the LAU 2 regions, of which 877 provide nonzero volumes. Either the remaining 227 regions have no arable land, or all straw is consumed by livestock farming. The northern and eastern
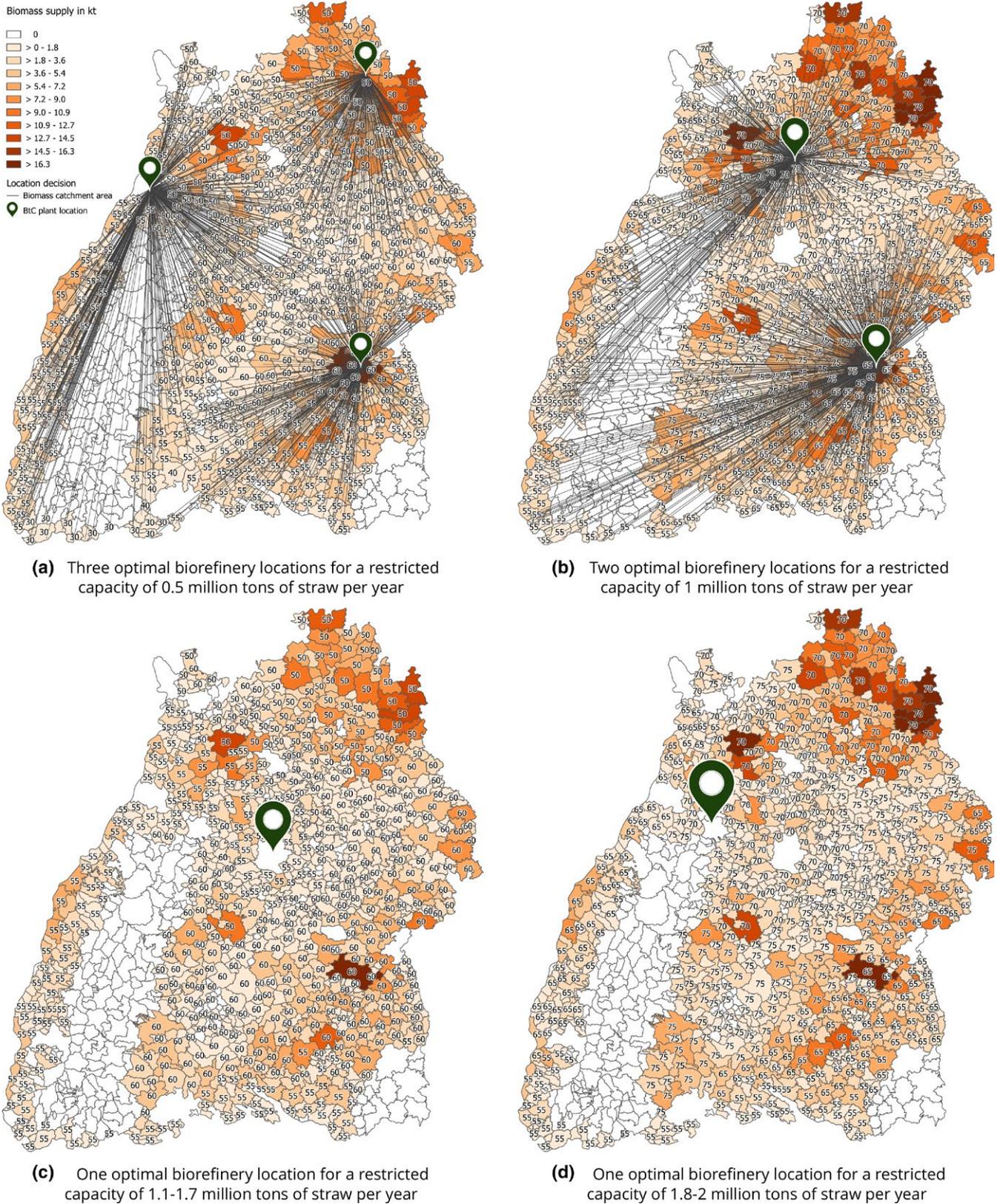
(a) Three optimal biorefinery locations for a restricted capacity of 0.5 million tons of straw per year

(b) Two optimal biorefinery locations for a restricted capacity of 1 million tons of straw per year

(c) One optimal biorefinery location for a restricted capacity of 1.1-1.7 million tons of straw per year

(d) One optimal biorefinery location for a restricted capacity of 1.8-2 million tons of straw per year

FIGURE 7 Modeling results of optimal biorefinery locations and straw supply prices at LAU 2 level for four capacity restriction scenarios (size of location marker is proportional to biorefinery capacity)

regions of Baden-Wuerttemberg provide higher quantities of straw supply in contrast to the western (Black Forest) and the southern (Allgäu) regions.

The centralized structure of the supply flow toward the city of Stuttgart is characterized by an average transport distance of approximately 100 km with the longest distance being

231 km. The modeled biorefinery produces 224 kt/year of lignin, 640 kt/year of glucose, and 365 kt/year of residual C5 sugars. By assuming a lignin price of 1,000 €/t (Bruijnincx, Weckhuysen, Gruter, & Engelen-Smeets, 2016; Rettenmaier et al., 2014; Smirnova & Zetzl, 2016; de Wild, Huijgen, & Gosselink, 2014), a glucose price according to the world market price of 350 €/t (EC, 2018a), and a C5 sugar price corresponding to 60% of the glucose price (Haase, 2012), a total profit of approximately 86 million €/year is obtained. The share of total costs consists of 10% for transportation, 25% for straw supply costs, and 65% of technology-related investment costs per year.

Figure 8 summarizes the modeling results of 18 distinct biorefinery capacities and the number of biorefineries implemented within the capacity scales (x-axis). The costs of transportation and straw supply as well as the total sales revenue for each restricted capacity are presented (y_1-axis). In addition, the average straw supply price is shown (y_2-axis).

Under the aforementioned product price assumptions, even small-scale biorefineries generate a profit. Furthermore, with growing capacities, the number of small-scale biorefineries increases to up to three with locations in the northern, central, and southeastern regions of Baden-Wuerttemberg (cf. Figure 7a,b). Limited by the maximum available straw quantity and starting from a capacity of more than one million t_{FM} of straw per year, one central biorefinery near Stuttgart has been selected (cf. Figure 7c). This location remains unchanged up to an input of 1.8 million t_{FM} with Pforzheim being the optimal location (cf. Figure 7d). Pforzheim and especially Stuttgart are located in the center of Baden-Wuerttemberg, and both have an excellent road transport connectivity. While the transport costs remain almost unaffected due to the robust central location choice, the straw supply price becomes significant with larger capacities. This critical price describes the optimal price-to-quantity ratio of straw supply and represents a threshold for an economic supply of approximately 50–60 €/t_{FM} on average (cf. Figure 4). Hence, instead of implementing a biorefinery of the largest possible

size, a capacity size is chosen, which valorizes a straw quantity that has the best price-to-quantity ratio. In the case of the optimal solution of 1.6 million t_{FM}, the average supply costs are 56 €/t_{FM}, as highlighted in Figure 8. In difference to the average straw supply costs, the variation of transportation costs lowers the overall profit, but does not affect the plant location decision.

In general, due to the need for large quantities of low-cost feedstock, the profitability of a large biorefinery is very sensitive to any increase in feedstock costs (Zimmer, Rudi, Müller, Fröhling, & Schultmann, 2017). This relationship between EoS of larger capacities and diseconomies of scale of higher supply quantities becomes relevant for biomass value chains on regional level, when transportation costs play a minor role (Richard, 2010). At a biorefinery capacity of larger than 1.6 million t_{FM}, the EoS are compensated by disproportionately increasing feedstock costs. Hence, higher capacities benefit the EoS at the cost of higher supply prices when transportation prices are irrelevant.

4 | DISCUSSION

The results of the study indicate the influences of different problems and trade-offs regarding the supply chain optimization of energetic (BtE) and material (BtC) biomass pathways. Biorefineries for material production are facing enormous investment cost and benefit significantly from cost digression that comes along with larger plant capacities. On the contrary, such concepts demand very high feedstock volumes whose provisioning becomes much more challenging with increasing plant size (Wang, Ebadian, Sokhansanj, Webb, & Lau, 2017). In addition, modeling of the agricultural straw supply shows significant effects of competition for the use of arable land. This competition results in a declining progression of straw supply curves at higher straw prices (>60 €/t_{FM}).

The straw supply curves, in general, are driven by the typical regional farm characteristics. In regions with a high share
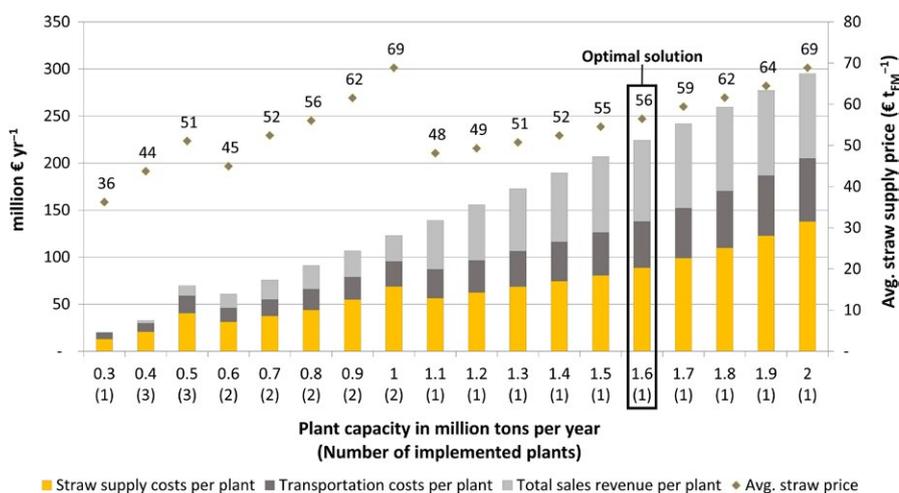

FIGURE 8 Results of restricted plant capacity model runs and optimal solution without restriction of plant capacity

of cropping farms such as AER 1, the farms adjust the cropping pattern for the sole profitability of the specific arable crops. In these regions, the farms start to provide straw when the costs of provision (baling, collecting, and on-field storage) and nutrient removal are covered by the sales proceeds. In the case of high straw prices, crop rotation shifts toward an extended grain production. Furthermore, because of higher straw yields, the production of spring grains is decreased in favor of increased winter grain cultivation.

In regions with extensive animal production, the supply curve increases less prominently (e.g., AER 6). This is explained by the competition of arable land for straw as feedstock and for livestock production. These regions are characterized by a higher profitability of the feed demand for livestock production than of the utilization of straw in BtE or BtC pathways. In contrary, the nutrient removal can be balanced to some extent by the farms' nutrient supplies through the purchase of feed that is returned to the field as manure. This reduces the demand for fertilizer required for replacing the nutrients and the humus removed through straw exploitation. Such representation of different contradictory effects reveals the advantage of agricultural farm models in the assessment of agricultural biomass valorization in the context of bioeconomy.

In the following, the modeled straw supply is compared with the findings by Gauder et al. (2011). They calculated a maximum straw production including the change in crop rotation of 2,326 kt_{DM} in Baden-Wuerttemberg, which corresponds to 2,705 kt_{FM} with a moisture content of 14%. EFEM models a maximum straw supply of 2,478 kt_{FM} without consideration of the additional demand for husbandry production, but includes an equated humus balance. However, considering the straw demand for a stable humus balance, the remaining supply calculated by Gauder et al. (2011) for BtE or BtC pathways is 842 kt_{DM}. This is only half the quantity of the modeled optimal feedstock supply. The difference in quantity is primarily explained by the additionally available options in EFEM to cultivate crops, such as intercrops, that have a positive effect on the humus supply.

A weakness in the presented model approach is the regional system boundaries of EFEM that do not allow the consideration of trade with the neighboring regions. Whereas the import of straw from Switzerland is probably negligible, the import from, for example, Bavaria is likely to have a significant impact on the straw supply in Baden-Wuerttemberg at a high straw price. The export of straw from Baden-Wuerttemberg to the neighboring regions, especially at higher prices, is not profitable and has therefore not been considered. However, such implementation of BtE or BtC value chains is most likely to be realized at country level, creating a competition across federal state borders. To address these issues, the regional study area should be expanded to at least the neighboring federal states in further studies.

Direct conclusions on the effects of location decisions of biomass conversion plants on the farms cannot be drawn yet due to the different spatial resolutions of the two models. Nevertheless, at a straw price up to 50 $€/t_{FM}$ as in the BtE scenarios, only the straw of the existing grain production is supplied to the particular valorization pathway. With an increasing straw price, the farms change the crop rotation to expand the cereal cultivation for an increase in straw production. This shift in crop rotation is to the detriment of silage maize and rapeseed, which are already being used in a BtE pathway (biogas, resp. biodiesel). However, the increased grain production due to the coupled production must additionally be offset against the reduced silage maize and rapeseed production in the evaluation of the total output. This trade-off is caused by the limited availability of arable land. Such aspects must be kept in mind when evaluating the contribution of the modeled biomass valorization pathways.

For further model extension, an additional risk premium to be paid to the farmers is intended to be introduced to cover realistic barriers, which affect the farmers' willingness to sell straw for one of the considered pathways (Glithero, Ramsden, & Wilson, 2013). The determination of premium prices, however, is extremely challenging. Furthermore, the integration of yield fluctuations of straw seems appropriate in order to consider the financial risks caused by shortages of feedstock supplies, for example, based on unfavorable weather conditions. Furthermore, perennial lignocellulosic feedstocks such as short-rotation coppice or miscanthus can also be integrated into the model linkage. In this context, miscanthus is a promising crop because of high biomass yields and a good environmental profile (Jørgensen, 2011). It is also suitable because it can grow on marginal land, which has no competition with the feed and food crop production (Lewandowski et al., 2016).

In order to promote straw for BtE and BtC valorization pathways, the focus on plant breeding could be redefined. In recent years, the focus of plant breeders has been mainly on the increase in grain yield, which generally reduces the straw-to-grain ratio. It might be useful to extend research on dual-purpose wheat crops for increasing the profitability of both straw as a feedstock and grain for food and feed production (Townsend, Sparkes, & Wilson, 2017).

Having a closer look at the economics of the lignocellulose biorefinery concept, the price of high-value lignin is the most decisive factor in the techno-economic analysis, because it only provides profitable solutions starting from a price of 700 $€/t$. Additionally, the lignin price is subject to an uncertainty as it ranges from 750 to 1,300 $€/t$ (Bruijnincx et al., 2016; Rettenmaier et al., 2014; Smirnova & Zetzl, 2016; de Wild et al., 2014). Hence, the finally implemented lignin price has a great influence on the future development of the BtC value chain.

When looking more closely at the results of the location optimization, the EoS crucially affect the profitability of the BtC pathway. The assumed EoS of the BtC biorefinery concept are based on scale-up factors from the literature up to a maximum of 2 million t_{FM} of straw supply per year. However, financial scale-up risks occur with larger capacities, which hamper the implementation of large-scale BtC concepts significantly (Castillo-Villar, Eksioglu, & Taherkhorsandi, 2017). Integration of such risk factors promotes small-scale concepts because of lower risk investments, but on the contrary reduces EoS of large-scale BtC concepts (Bruins & Sanders, 2012). Additionally, the size of a biorefinery can have a significant impact on emissions and the regulatory requirements (Eberle, Bhatt, Zhang, & Heath, 2017). The technology readiness level of the proposed lignocellulose biorefinery concept still has not surpassed the pilot stage; therefore, it is impossible to estimate emissions realistically. Moreover, the requirements for emission reduction measures depend on regional environmental conditions and policy regulations. Acceptance by the local society could also interfere with the location decision and should be considered in future works (Lee, Loveridge, & Joshi, 2017).

Numerous studies highlight the application of decentralized biomass value chain concepts with locally separated pretreatment, primary and secondary refining processes (Kudakasseril Kurian et al., 2013; Lin et al., 2016; Sokhansanj et al., 2010). Such value chain structures are characterized by the decision of optimizing the pretreatment plant location in addition to the conversion plant location. However, this requires multi-echelon modeling approaches, which enable an advanced problem consideration.

EoS are an important factor in location optimization of biomass conversion plants. Capital-intensive technologies such as the lignocellulose biorefinery (BtC) are characterized by a significant impact of EoS on the profitability forming centralized valorization structures. Economies of Scope, on the contrary, are primarily affecting the downstream value chain leading to cost reductions through product diversification. The assessment of valorization routes of lignin and organosolv sugars along the downstream processes is a key aspect of future research. For bioenergy generation (BtE), such effects are less important. Policy incentives such as surcharges, which favor decentralized BtE structures with medium-sized combustion capacities, are rather crucial.

In order to meet the requirements of the bioeconomy, the ecological footprint of biomass value chains must be improved in comparison with that of fossil-based value chains. Ecological impacts are crucial for fulfilling the role of the biomass valorization pathways for the bioeconomy. For that reason, environmental effects such as GHG emissions should be integrated and a Life Cycle Analysis applied to evaluate the ecological performance of biomass conversion technologies. However, the integration of GHG emissions into an optimization model requires advanced modeling techniques such as multi-objective optimization. One approach, that is, the augmented epsilon-constraint method, seems promising and is currently being integrated (Rudi, Froehling, Zimmer, & Schultmann, 2017). Another model enhancement is the increase in the spatial resolution of biomass supply based on land use maps, and the inclusion of crop residues other than cereal straw.

In summary, the presented linkage between an agricultural farm model (EFEM) and a biomass conversion plant location optimization model (BIOLOCATE) elucidates the trade-off between economies of scale and increasing feedstock supply costs in southwest Germany. The results highlight the advantages of linking two models for the techno-economic analysis and optimization of biomass-to-energy (BtE) and biomass-to-chemical (BtC) pathways while taking into account technological economies of scale (EoS) and regional price-sensitive agricultural production.

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SUPPORTING INFORMATION

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