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Trade-offs in biomethane production by substrate mixture optimization under German market conditions

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Abstract

Background New regulations and market conditions in Germany affect the profitability of biomethane upgrading as a repowering option for existing biogas plants following on-site CHP utilization. These conditions present trade-off challenges between higher sustainability requirements, maintaining production capacity and new revenue opportunities. Optimization methods, such as linear programming (LP), are essential for determining the ideal substrate mixture and profitable solutions amidst multiple market conditions, plant-specific process constraints, and substrate properties.

Methods We updated a substrate mixture optimization model within an assessment framework for the repowering of existing biogas plants (BGPs), which focuses on the operator's perspective. By integrating multiple German biomethane markets for various BGPs, we assessed changes in the substrate mixture, GHG emissions, contribution margins, and constraint parameters to derive conclusions for operators and future framework design.

Results Integrating market revenues and constraints can increase contribution margins by 12–55%. Additional gains can be achieved by considering multiple markets simultaneously but limited to a few BGPs. The plant-specific LP solution space and used benchmark market are decisive. The former limits the potential of high substrate-specific contribution margins, which has a significantly higher impact than the relation between plant-specific characteristics and process constraints. The advanced fuel market is currently the lead market for biomethane, incentivizing GHG-emission extensive substrates, decreasing gas production and GHG emissions but increasing levelized cost of energy (LCOE) and partially CO_2 abatement costs.

Conclusions The key to improve profitability and to supply an increasing biomethane demand while fulfilling new requirements is a large LP solution space. Increasing market options, substrate availability, and digestion system capacity achieve this on the operator's side. Policy makers could reduce normative requirements such as the maize cap or double counting of advanced fuels and favor high but uniform GHG requirements. Operators can prepare robustly for the future substrate mixture by adding digester volume and pre-treatment tech, ensuring long-term and diverse substrate availability, and contracts with flexible components. Although current market conditions can improve specific GHG emissions, they do not necessarily increase manure usage when other options, such as straw, are viable. Other regulatory support systems will be required to do so.

Keywords Biomethane, Substrate mixture, Optimization, Biogas plants, GHG quota, GHG reduction requirements, Variable gas costs, Linear programming

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Background

Status quo of biogas and biomethane in Germany

As the energy transition progresses further, new framework conditions affect existing biogas plants and their future operations. Existing support schemes, such as the German Renewable Energy Sources Act (EEG), are modified in favor of more market-driven solutions and might phase out eventually. Likewise, frameworks, such as the EU's revision of the Renewable Energy Directive (REDIII) or the RepowerEU strategy, state new production targets or increase sustainability requirements regarding the reduction of greenhouse gases (GHG) [1].

In Germany, BGPs traditionally supply electricity via on-site combined heat and power (CHP) utilization. In these, the current substrate mixture is made up 50% by energy crops and 50% by manure. Energywise energy crops deliver about 75% [2]. For existing biomethane upgrading plants, which mostly deliver the EEG CHP market, the share of energy crops is even higher. Across all BGPs, including biomethane production, maize silage delivers more than 50% in energetic terms.

Due to the versatile features of biogas, utilization likely shifts towards the supply of heat, e.g., for high-temperature processes [2], and transport fuels, e.g., for heavy-duty vehicles or aviation and shipping [3]. Since decarbonization through electrification is particularly difficult in these areas, biomethane utilization is a suitable option [4]. In the electricity sector, utilization will tend to stagnate but will be more flexible and targeted [5–7]. This utilization shift is also in line with the German energy policy strategy for future biomass use [8] and the role of gaseous fuels in the energy system transition [9].

The utilization shift requires a strategic switch to biomethane production and concerns the possible extension of the operation of existing BGPs after the initial time 20 years within the EEG support scheme. Since an extension is technically feasible and associated with decreased capital-related costs, the new framework conditions call for repowering and follow-up concepts. One such concept is the switch to biomethane upgrading, i.e., CO_2 removal from biogas. Biomethane upgrading would be particularly advantageous in the case of insufficient heat utilization of on-site CHP [10]. This switch is also part of a development strategy for bioenergy proposed by Thrän et al. [11] and the first phase of a transition to a green gas supply [12]. Matschoss et al. [13] estimate the potential of switching to biomethane upgrading at 24.9 TWh_{HHV}. Including existing and new upgrading plants, the total biomethane potential in Germany is estimated at 90–118 TWh_{HHV} [14].

At the same time, the utilization shift is accompanied by a feedstock shift towards perennial crops and biomass residues and waste streams such as straw. As the potentials of these biomass streams might be fully exploited the resulting biogas and biomethane production will be limited by the availability of land to produce of energy crops [15, 16].

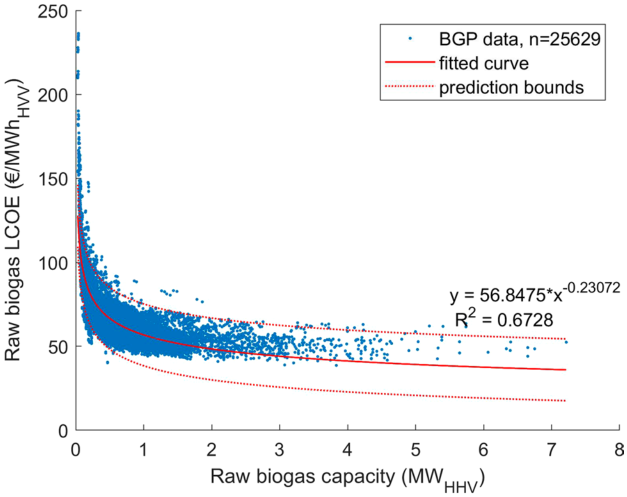

Fig. 1 Modeled LCOE of biogas over the average production capacity; aggregated data for different repowering concepts ($n = 3$) and scenarios ($n = 3$), capacities below 30 kW are excluded, based on [27]

Challenges and opportunities regarding biomethane profitability and markets

Levelized cost of energy for biomethane

High biogas costs, caused by the substrate mixture-related costs, are one of the major challenges for the switch to biomethane upgrading. Since economies of scale favor larger BGPs [17], high biogas costs mainly apply to smaller BGPs, below 1 $MW_{HHV,biogas}$. These represent most BGPs with on-site CHP utilization operating in Germany (Fig. 1). In contrast, the average capacity of the current upgrading plants is at 6.320 $MW_{HHV,biomethane}$ [18]. The specific upgrading costs for smaller capacities are also high, typically above 20 €/MWh_{HHV} [19]. The resulting levelized cost of energy (LCOE) for biomethane makes it challenging to compete with historically low natural gas (NG) prices in the range of around 20 €/MWh_{HHV}. The price spike during the energy crises of 2021 and 2022 [20] made biomethane competitive only for a short time. Reducing substrate-related costs is crucial for profitability, while substrate diversification can also reduce associated risks.

However, smaller BGPs have a high potential for GHG emission reduction due to their high content of manure [21] and their integration into local agriculture. Recent research has focused on the development and cost reduction for small-scale applications to facilitate access to these valuable potentials [19, 22, 23]. Among the upgrading technologies, membrane upgrading shows economic advantages with low specific upgrading costs [24], leading to market share increases [25]. However, it might not be the best option from an environmental standpoint [26].

High CO_2 price levels strongly favor the profitability of biomethane or other green gases such as hydrogen. Such high CO_2 price levels in all sectors are necessary to meet climate targets [28] and can induce a high price range (100 €/MWh_{HHV}) for green gases and an overall market share of 50% [29]. In such a price range, biomethane would be competitive with other green gases and a viable option for a large segment of existing BGPs. Biomethane is also advantageous due to its technological readiness and carbon availability, making it attractive for many industrial processes. Even assuming cost reductions for green gases (compare the determined time series in Table 12 in Appendix), biomethane will likely remain one of the cheapest options. It also shows lower LCOE than synthetic NG from solid biomass [30]. As a result, the demand for biomethane is expected to grow [31]. Biomethane potentials are the first to be fully exploited [29], and future gas markets are likely to include domestic biomethane [32].

Fragmented policy support for biomethane markets

Another challenge is that the non-uniform treatment of fuels in different sectors hinders urgent investment with long investment cycles. Härtel and Korpås argue that successful decarbonization requires the harmonized treatment of fuels across energy sectors and a congruent framework condition but note that such cross-sectoral market designs are challenging [33]. One issue is that the required CO_2 price range is very different in each sector, e.g., the EU ETS sector requires much lower prices than transport and buildings. Hence, complementary policy instruments are required in addition to carbon pricing [28].

Biomethane itself is used in several markets in Germany. These are the utilization in biomethane CHP units under the EEG support system, the substitution of NG in the fuel and heat market, and international trade (see Table 9 in Appendix for an overview). Next to these, there is also market option for material use, which might become a more important market in the future [34]. The highest carbon prices are currently found in the fuel market due to the tightening of the GHG reduction quota [35]. Prices are especially high for GHG emission extensive biomethane and changes the incentivization of the underlying substrate mixture. Regular CO_2 prices range between 240 and 525 €/tCO_2-eq [36]. However, the NG fuel market volume [compressed and liquified NG (CNG/LNG)] is small compared to other biomethane markets. Current biomethane sales comprise about 1/3 of the market volume of 3 TWh_{HHV}. Still, the methane fuel market is expected to grow, with forecasts for the LNG market ranging from 9.7 to 32.5 TWh_{HHV} in 2030 [37], of which half could be covered by biomethane [38]. The main driver is the requirements of the RED II for advanced fuels. Other emission benefits, e.g., for NO_x and temporary toll exemptions for trucks until 2023, have further boosted LNG infrastructure and the fleet of heavy-duty vehicles [39]. Also, large industrial and oil companies are looking for new business opportunities and are driving efforts to replace fossil LNG [40, 41]. In addition to the fuel market, many ongoing developments are driving further demand for biomethane:

- Due to the strong political support mentioned above, the European market for biomethane is growing [42], while cross-border exchange is increasingly facilitated [43].
- Due to cost advantages, centralized biomethane usage in CHP units and combined cycle gas turbines (CCGT) may experience growing demand in the future [15].

Research questions and objectives

The multiple biomethane markets could be served in parallel or alternating depending on the contract situation and revenue options. These markets differ significantly in demand (market volume), prices and willingness to pay, volatilities and risks, and regulatory drivers and requirements, e.g., GHG emissions. Decision making regarding an optimized biogas production becomes even more complex when additional export markets, long-term planning, and contracts are considered. The challenge is to find the optimal trade-off between meeting the non-uniform requirements and incentives of different markets while taking into account process restrictions and substrate costs. From the regulator's perspective, there is a trade-off between setting ambitious sustainability goals and expanding the supply of renewable biomethane energy, ideally across multiple markets simultaneously.

One method to do so is to optimize the substrate mixture via linear programming (LP). LP optimization models can also be used to reduce LCOE and increase profitability, as applied in [44] regarding the assessment of alternative crops or in [45] regarding the effects of different process restrictions. The integration of different biomethane markets with their specific revenue and requirement structure into such models and the effects of the subsequent optimal substrate mixture decision from the operator's perspective is missing in current research. Hence, we developed and applied a substrate mixture optimization model for a wide range of German BGPs to achieve the following objectives and provide recommendations for operators and good climate policy:

1. Identify and analyze the effects of different market requirements and revenues …
    a. on the substrate mixture, variable biogas costs, and related GHG emissions
    b. on the limiting constraints and process implications.
2. Assess profitability gains in contribution margin (revenues minus variable costs) and net present value (NPV) …
    a. by considering single markets, e.g. biomethane as a transport fuel and the GHG quota market
    b. by considering multiple markets (integrated optimization)
3. Assess relations and changes in substrate mixture and market shares caused by changes in revenues and requirements (non-uniform market conditions) to conclude the future design of market conditions.

By fulfilling these objectives, we try to gain new and additional insights on the trade-offs in the future biomethane supply by biogas plants.

Methods

To achieve the objectives and derive robust results, we are mainly using an LP model for the substrate mixture optimization applied to a wide range of BGPs in Germany. This model is integrated in an existing model framework for the assessment of biogas repowering, referred to as BGP-RepoMod. In the first method section we shortly introduce and describe this model. In the main method section, we present major model details regarding the substrate mixture optimization which are newly integrated within the scope of his study. These contain the objective function, constraints, and related inputs of the substrate mixture optimization. This is followed by the description of the analyzed market variants, and model settings used to determine the potential of integrating revenues from single or multiple markets. The biomethane technology modelled and the update of the BGP-RepoMod scenario framework are also described. Afterwards, a methodology update for selecting representative reference BGPs (REF BGPs) is given which is used for the presentation of results. Lastly, key performance indicators (KPIs) such as the NPV or CO_2 abatement costs are introduced which are used in the final assessment.

Overview on the existing model framework

The BGP-RepoMod was initially described in [46]. It has been further developed in [27] and [47] concerning the integration of additional repowering concepts, regions, and extended scenario framework capabilities. An overview of BGP-RepoMod is shown in Fig. 2. To model the heterogeneity of BGPs, the model follows a plant-specific bottom-up approach instead of normatively specifying reference-type plants. It is well scalable to any given size of the primary input data. Each step and model function is calculated individually and independently for each BGP.

The primary model input consists of the merged EEG plant master and transaction data released by the German Transmission System operators (TSO) and several monitoring studies and surveys on the regional BGP structure. The model consists of three main model modules and one central scenario evaluation module (E1), which includes the simulation of a simplified EEG tender process (not part of this study). The substrate analysis module (M1) and Status Quo configuration module 2 (M2) are conducted consecutively and determine the status quo of each BGP as the primary input for the integrated repowering analysis module 3 (M3). M3 consists of several submodules: the integration of scenario parameters and settings of the repowering measures, an optional substrate mixture optimization, the component and annualwise mass-, energy-, and GHG-emission balances, the CHP dispatch optimization, and economic evaluation. All results are integrated over the defined period under review. The effects of the implemented measures and scenarios are assessed using specified KPIs. A decision KPI can be used to determine if a BGP extends operation or is decommissioned according to a specified criterion. Although BGP-RepoMod focuses on the operator perspective, this allows for comparing the BGP development from different societal goals (e.g., a macroeconomic perspective). The current study focuses on the substrate mixture optimization model as part of M3.

The substrate mixture optimization model

In its previous version [27], the substrate mixture optimization model could only optimize cost while satisfying a single market's technical and regulatory requirements. In the following the details of the model updates regarding the market revenues and restrictions are given.

The model for optimizing the substrate mixture is a mathematical model of linear programming. As with the

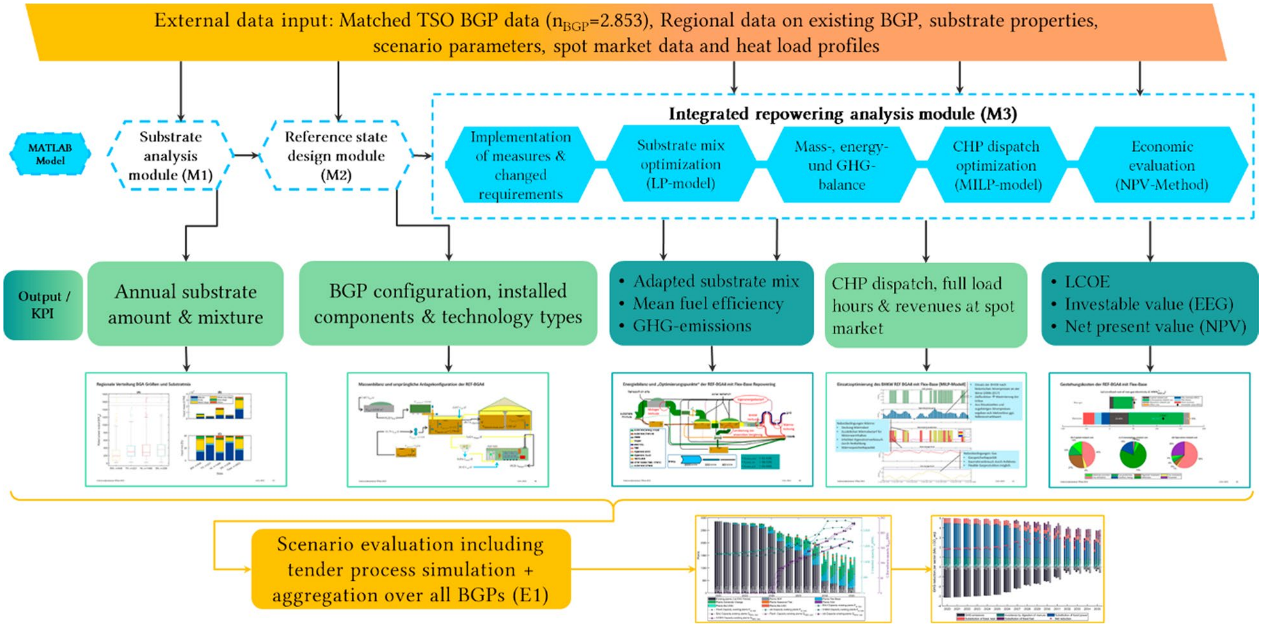

Fig. 2 Overview of model framework BGP-RepoMod in which the substrate mixture optimization is integrated (updated from [27])

rest of the BGP-RepoMod, the substrate mixture optimization is formulated in MATLAB. It is solved using MATLAB's *linprog* function [48] and applied for each BGP individually. The objective of the substrate mixture optimization is to minimize the cost of the substrate mixture or, in the case of revenues, to maximize the contribution margin of biogas production. At the same time, the model must meet the regulatory requirements of different markets and consider plant-specific conditions and process restrictions. The general structure of this LP model is given in the following equation:

$$\min f\left(x_{ij}\right) \text{ such that} \begin{cases} A * x_{ij} \leq b \\ \mathrm{lb}_j \leq x_j \leq \mathrm{ub}_j \end{cases}, \qquad (1)$$

where $x_{i,j}$ represents the substrate variables that equal the yearly mass input of each substrate j in the market i. This study considered 17 different types of substrates plus the optional variable of the recirculation material (see the supplied list of substrates and their property data in Additional file 1). Each substrate has its specific properties such as total solids (TS_j) or volatile solids (VS_j), energetic and volumetric standard methane yields ($\mathrm{SMY}_{e/v,j}$), specific costs (c_j), GHG emissions factors (GHGe_j), substrate groups categories, i.e., energy crops, and fugate factors ($f_{\mathrm{fug},j}$). The plant-specific upper (ub_j) and lower bounds (lb_j) equal the maximum and minimum yearly mass input per substrate. In this study, only manure substrates have an upper bound in relation to the determined reference mix and thereby a restricted availability (see Table 1).

All constraints of the LP model are considered as inequality equations. In addition to regulatory market requirements and process restrictions, there are plant-specific and normative constraints (Table 1). There are 11 constraints, which may be applied market-specificwise or cumulative for all substrates used in the plant. Depending on the constraint, plant-specific characteristics such as the volumes of the digester, gastight system, or digestate storage are used in addition to the substrate-specific properties.

Objective function

The objective function of the LP model is to minimize the yearly variable gas production costs, including possible substrate-specific and gas value-related revenues. Revenues greater than the variable substrate costs equal maximizing the contribution margin of gas production. The underlying objective equation can be formulated as follows:

$$\sum_{i=1}^{m}\sum_{j=1}^{n}\left(C_j - \left(\mathrm{GHGe}_{\mathrm{fossil,\,ref}} - \mathrm{GHGe}_j\right) \times \frac{P_{\mathrm{CO}_2 i}}{1000} \times \mathrm{SMY}_{\mathrm{e},j} - P_{\mathrm{gas},i} \times \mathrm{SMY}_{\mathrm{v},j} \times \frac{\mathrm{LHV}_{\mathrm{CH}_4}}{1000}\right) \times x_{ij}. \qquad (2)$$

Table 1 Constraints, settings of boundary conditions, and revenues of the main markets, including no revenues variants

Type	Constraints	Class	Unit	Boundary conditions for main markets						
				M1-GHG-Q NoRev	**M2-EEG NoRev**	**M1-GHG-Q**	**M2-EEG**	**M3-NG**	**M4-GreenG**	**M5-Adv.GHG-Q**
Plant-specific	Methane production	Min	Nm^3	Plant-specific REF values (Table 3)		–				
	Digestate storage capacity (DSC)	Min	d	Plant-specific REF values (Table 3)						
Regulatory	$HRT_{gastight\ system}$	Min	d	0	150	0	150	0	0	0
	GRT vs. fossil reference[a]	Max[a]	%	-77^b	-80^b	-77^b	-80^b	0	-80^b	-77^b
	Maize cap	Max	% of the mix	0	36^b	0	36^b	0	0	0
Process	$TS_{In,\ digester}$	Max	%	36						
	$TS_{Out,\ digester}$	Max	%	15						
	OLR	Max	kg VS/m^3 d	6						
	$HRT_{digester}$	Min	d	Plant-specific REF values						
Normative	Upper bounds for substrate groups	Max	% of mix	EC: 80%, Gras: 50%, Residues: 20%, Manure: 100%						EC: 0%, Gras: 0%, Residues: 20%, Manure: 100%
	Upper substrate-specific bounds	Max	% of mix	See substrate property data in Additional file 1						
	Lower/upper bounds manure	Max/Min	tFM/a	0% of the REF input/130% of the REF input						
Revenues	Revenues gas	–	€/MWh	0	0	9^b	106^c	35^b	118^b	9^b
	Quota price	–	€/tCO_2-eq	0	0	350^b	0	0	0	700^b

[a] The model uses specific values, e.g., in kg CO_2-eq/MWh, as an upper bound for the GHG emissions

[b] Plant-specific values can differ. Here only average values are given. Plant-specific means are based on time series assigned to each BGPs under its extended operation period. Time series are given in Table 12 in Appendix

[c] Based on a pricing model for biomethane CHP units in the EEG, see Additional file 2 for details

Constraints

All constraints are formulated as inequalities. In general, constraints related to the process, plant-specific and normative types are market independent. All equations for the constraints from Table 1 are given below. In these, m and n represent the number of markets and substrates. Equation (3) gives the constraint for methane production. It can be deactivated by setting the minimum methane production to zero:

$$-\sum_{i=1}^{m}\sum_{j=1}^{n}\mathrm{SMY}_j \times x_{ij} \leq -\mathrm{Methane\ Production}_{\min}. \tag{3}$$

The constraint regarding the minimum digestate storage capacity (DSC) is given in (4) and is dependent on the available volume of the digestate storage tank(s):

$$\sum_{i=1}^{m}\sum_{j=1}^{n}\left(\frac{f_{\mathrm{fug},j} \times \mathrm{DSC}_{\min}}{365 \times \rho_{\mathrm{average}}}\right) \times x_{ij} \leq V_{\text{digestate storage tank}}. \tag{4}$$

Equations (5) and (6) set the constraints for the maximum TS content in the input mix and digester outflow, respectively. $\mathrm{TS}_{\mathrm{out}}$ values are calculated via the fugate factors and are given in the substrate property data in Additional file 1:

$$\sum_{i=1}^{m}\sum_{j=1}^{n}\left(\mathrm{TS}_j - \mathrm{TS}_{\max}\right) \times x_{ij} \leq 0, \tag{5}$$

$$\sum_{i=1}^{m}\sum_{j=1}^{n}\left(\mathrm{TS}_{\mathrm{Out},j} - \mathrm{TS}_{\mathrm{Out,max}}\right) \times x_{ij} \leq 0. \tag{6}$$

The process parameters for the organic loading rate (OLR) and the hydraulic retention time (HRT) are given in Eqs. (7) and (8). The $\mathrm{HRT}_{\min}$ constraint for the gastight system is expressed similarly to Eq. (8), using the gastight system's volume and $\mathrm{HRT}_{\min}$. As $\mathrm{HRT}_{\min}$ in Eq. (7) cannot be set to zero, it is set to minimal values in cases where no such requirement exists

$$\sum_{i=1}^{m}\sum_{j=1}^{n}\left(\frac{VS_i}{365 \times V_{\mathrm{digester}}}\right) \times x_{ij} \leq \mathrm{OLR}_{\max}, \tag{7}$$

$$\sum_{i=1}^{m}\sum_{j=1}^{n}\left(\frac{1}{365 \times \rho_i \times V_{\mathrm{digester}}}\right) \times x_{ij} \leq \frac{1}{\mathrm{HRT}_{\text{digester, min}}}. \tag{8}$$

The GHG emission reduction target (GRT) constraint relative to the fossil reference is regarded via Eq. (9) for each market m. The GRT in (9) is calculated via the relative target in Table 1 and the market-specific fossil references. The latter is set to 338 kg-CO_2/MWh for the fuel markets, 256.9 kg-CO_2/MWh for electricity,[1] and 288 kg-CO_2/MWh for heat, according to the REDII [49]:

$$\sum_{j=1}^{n}\left(\mathrm{GHGe}_j - \mathrm{GRT} \times \mathrm{SMY}_j \times \mathrm{LHV}_{\mathrm{CH}_4}\right) \times x_j \leq 0. \tag{9}$$

Constraints regarding the substrate mixture's minimum or maximum relative share, such as the maize cap, are integrated via Eq. (10). Other relative constraints for substrate groups, such as grass or individual substrates, work the same way as the maize cap:

$$\sum_{j}^{\text{Maize cap substrates}}\left(1 - \mathrm{Maize\ cap}_{\max}\right) \times x_j + \sum_{j}^{\text{Others}} -\mathrm{Maize\ \ cap}_{\max} \times x_j \leq 0. \tag{10}$$

The recirculation variable works just like any other substrate variable but is excluded from most constraints by setting its substrates properties accordingly. The recirculation is mainly involved in the TS-related constraints. In the example of the maize cap, this means that the recirculation mass does not count towards the summation of the other substrates or the total mass input.

Main model variants and settings

Eleven main variants of the substrate mixture optimization model were calculated. The reference substrate mixture (REF), which is not the result of the optimization but of the BGP-RepoMod Modules 1 and 2, is also compared. The boundary conditions of the constraints and revenues for each market are shown in Table 1. There are five main markets:

1. Fuel and GHG quota in the transport sector (**M1-GHG-Q**),
2. Biomethane for CHP plants in the EEG (**M2-EEG**),
3. Substitute for fossil NG (**M3-NG**),
4. Generic green gas market, e.g., for industrial heat (**M4-GreenG**),
5. Advanced fuel and GHG quota as a submarket in the transport sector (**M5-Adv.GHG-Q**),

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[1] For the conversion of the fossil reference for electricity an average electric efficiency of 39% is assumed. Higher efficiency rates would therefore lower the GRT.

Table 2 Overview of the sensitivity analysis, its varied parameters, and parameter range

Primary sensitivity parameter	Secondary sensitivity parameter	Applied market variants	Range of primary sensitivity parameter	Range of secondary sensitivity parameter
Gas price in M2-EEG	M1-GHG-Q GHG quota price	M2-EEG and M1–2	50–180 €/MWh (44 steps)	150–450 €/tCO$_2$-eq (4 steps)
Gas price in M3-NG		M3-NG and M1,3	30–200 €/MWh (44 steps)	
Energy crops costs	Market variants	M1-GHG-Q NoRev, M1-GHG-Q, M1–2, M1,5, M1–5	0–100% (10 steps)	–
Non-energy crops costs				
GRT in M1-GHG-Q	M2-EEG and M3-NG gas price	M1–2 and M1,3	−65 to −95% (10 steps)	100–160 €/MWh and 60–180 €/MWh (4 steps)
GRT in M2-EEG	M1-GHG-Q GHG quota price	M2-EEG, M1–2		150–450 €/tCO$_2$-eq (4 steps)

In addition to the main five markets, further model setting variants with their own conditions were considered, which include the integration of multiple markets. For example, the variant **M1–5** combines the main markets M1-GHG-Q to M5-Adv.GHG-Q, while **M1,5** combines only those two markets. Of the main markets, only M1-GHG-Q and M2-EEG are analyzed as single markets. An overview and detailed description are given in Appendix Table 10. In model variants without revenues, such as **NoRestrict**, **M1-GHG-Q NoRev**, and **M2-EEG NoRev**, the minimum methane production constraint is active to enforce production. Otherwise, production would be zero as this is cost optimal. The model can gradually relax this constraint and reduce the methane production target, to find feasible solutions in case of too tight process constraints. In the case of M5-Adv.GHG-Q, the normative constraint for the upper bound of certain substrate groups was shifted into the regulatory constraint in such a way that the energy crops and grass were not allowed to be used. In the case of M5-Adv.GHG-Q, the normative constraint for the upper bound of certain substrate groups transforms into a regulatory requirement and the usage of energy crops and grass is not permitted. If specific regulatory requirements such as the maize cap do not apply in a market, they are switched off by setting the boundary conditions to zero, to values close to zero or to very large values, e.g., in the case of the GRT.

Next to these market variants, six sensitivities were calculated for substrate costs, selected market revenues and constraints (GRT). As shown in Table 2, these sensitivity variations were applied to only a subset of the market variants, with the applicability depending on the parameter varied. Single market variants, such as M2-EEG, are used as benchmarks to assess the benefit of the integrated market optimization. The classification of the substrates into energy crops and non-energy crops is given in the substrate property data in Additional file 1. In addition, static values for prices and GRTs are used instead of plant-specific time series (see values in Table 12 in Appendix).

Biomethane upgrading concept and framework settings

As the study focuses on biomethane markets, only membrane upgrading via membrane technology and grid injection as a repowering concept and one scenario framework are assessed in this study. Regarding the modelling of the technology no changes were made in relation to [27]. It is assumed that the total biogas capacity is upgraded, and the CHP unit is replaced by a two-stage membrane upgrading unit. The biomethane is then injected into the local NG grid. Due to the high operating pressure of the membrane process (8 bar), less gas compression is required for injection into the gas grid. Gas compression is also used to recover heat and supply internal heat demand. The distance to the NG grids is based on an on a fixed random sample of exponential distribution of about 3 km [19]. Due to the still high amounts of methane in the flue gas, a flue gas cleaning process with lean gas burners and heat recovery is assumed. The grid and a wood boiler supply the process electricity and the remaining heat demand on-site.

The main economic and regulatory framework data in relation to [27] was updated. It consists of the time series for price and GHG reduction targets presented in Table 12 in Appendix. In addition, there are basic framework settings for BGP-RepoMod concerning technical adjustments and progress. First, no further changes are assumed for the extended operation period with regard to the components of the biogas production, such as digesters. An exception is the coverage of open digestate storage tanks, if applicable. The new resulting digestion volume of the gastight system is considered in the substrate mixture optimization model. The effects of the coverage, such as capital costs or lower on-site GHG emissions, are modeled. Second, a renovation rate of 20% of the initial investment is assumed for components with a lifetime greater than 20 years and a reduction of investments for new upgrading technology of 0.3%/year. Finally, an annual substrate price increase rate of 4% is assumed for

Table 3 Main plant parameters of selected representative REF BGP and their corresponding reference clusters

Plant parameter	Unit	REF BGP1	REF BGP2	REF BGP3	REF BGP4	REF BGP5
Year of initial operation	–	2006	2015	2005	2007	2005
Region	–	SN	BW	NI	NI	BW
Rated power output	kW$_{el}$	470	73	275	675	278
Installed capacity	kW$_{el}$	530	75	600	865	350
Reference methane production	MWh$_{LHV}$	10,521	1751	6138	14,804	5158
Manure share	%	77%	82%	41%	14%	18%
Energy crops share	%	9%	10%	36%	47%	54%
Other substrates share	%	14%	7%	23%	39%	28%
HRT$_{\text{gastight system}}$	d	60	224	82	122	95
HRT$_{\text{digesters}}$[a]	d	40	51	75	112	89
Digester volume	m^3	3600	718	1775	4712	1387
Digestate storage[b]	m^3	14,521	2546	3818	3801	2395
Digestate storage capacity	d	252	196	198	197	199
Number of BGPs in the same cluster	–	206	456	195	338	202

[a] Difference between HRT$_{\text{gastight}}$ and HRT$_{\text{digesters}}$ for open digestate storage is explained by different densities ($\rho_{\text{digesters}} \neq \rho_{\text{digestate}}$) and input relation (HRT$_{\text{digesters}}$ regards recirculation)

[b] Includes volumes of pretank and external digestate storage tanks

Table 4 Key performance indicators for the concluding assessment of the substrate mixture optimization

Dimension	Parameter	Unit	Description
Economic (operator)	LCOE	€/MWh	Discounted, the specific production cost for energy (biomethane) of the period under review, including all relevant capital-related costs
	NPV	€/MWh	Discounted, specific revenues under market conditions minus LCOE
Macroeconomic	CO$_2$ abatement costs	€/t CO$_2$-eq	Difference of costs to fossil reference related to the difference in GHG emissions
Environmental	GHG-emissions	kg CO$_2$-eq/MWh	Total GHG emissions, including credits to the main energy product
	Net GHG reduction potential	%	Net GHG reduction (= gross reduction minus GHG emissions linked to biogas production) vs. a fossil reference

silages (maize, whole crop and grass) and grain, 1% for manure, and 1.8% for all other substrates.

Characterization of the selected reference BGP (REF BGP)

Since the BGP-RepoMod is run for a large data set of 2853 BGPs, REF BGPs are clustered and selected to illustrate plant-specific results and differences between them. Here, an update of the methodology in [27] is applied by changing the type and reduce the number of characteristic parameters describing the existing BGPs with a manageable amount of REF BGPs. We neglected the previously used regional and heat usage parameter, as these two parameters are less or not relevant in the context of biomethane upgrading. The resulting characteristic parameters are the rated power output, the substrate mixture in the form of manure share, and the digester volume. Each parameter refers to the reference state, i.e., the output of BGP-RepoMod modules 1 and 2. In comparison with [27], the introduction of the digester volume serves as relevant parameter in calculating several constraints, such as the OLR. It is thereby relevant to the substrate mixture-dependent gas production capacity.

For each parameter, a clustering formation was applied that divides all BGPs in the database into a fixed number of classes of equal frequency. Here the number of classes was also set to three (see Table 12). Combining different classes for all characteristic parameters leads to 27 (=3×3×3) clusters. The number of BGPs within the clusters varies between 0 and 456. Five reference clusters (with more than 190 BGPs) were chosen, reflecting almost 49% of all the studied BGPs ($n_{BGP}=2853$). One BGP was selected from each of these five clusters, whose characteristic parameters were closest to the mean values of the respective cluster. Thus, the five designated REF BGPs (Table 3) represent their clusters and were used to show and compare the results on the plant level.

Key performance indicators

Next to the NPV and contribution margin, LCOE, CO_2 abatement costs, the specific GHG emissions and net GHG reduction potential are used as KPIs (Table 4). These allow further conclusions to be drawn about the functioning of different markets' incentives and the utility of requirements, e.g., in environmental or macroeconomic terms. In the calculation of the LCOE and NPV, all further costs in the biomethane production besides the substrate-related costs are considered. For example, these cover, capital-related costs such as renovation of existing fermenters, replacement of components such as agitators and the investments in the biomethane upgrading technology (see [27, 46] for details). Compared with GHG emissions of the substrate mixture optimization, the GHG emissions calculated in Module 3 of the BGP-RepoMod also contain on-site emissions, e.g., due to methane losses and indirect GHG emissions linked to electricity consumption. These differences are also considered in calculating the actual GHG quota revenues and the NPV. The CO_2 abatement costs are accessed to compare the operator's perspective with the macroeconomic one, independent of market demands and specific revenues. The net GHG reduction potential and the CO_2 abatement costs are solely based on fuel as a fossil reference. The costs are assumed to be 51 €/$MWh_{fossil\ fuel}$ with a price increase rate of 1.67% per year. The CO_2 abatement costs are calculated only for the fuel market (M1-GHG-Q and M5-Adv.GHG-Q).

Results

We present results derived directly from the substrate mixture optimization model or module 3 of the BGP-RepoMod. The focus is on substrate mixture optimization, which gives information on the optimal substrate mixture, variable costs, GHG emissions, contribution margin, and resulting production volumes. The limiting constraints for individual REF BGPs and clusters are discussed to identify potential areas for technical adaptation and improvement. Market shares and gains in contribution margin are explored to show the impact of different market conditions and the benefits of integrated revenues of single or multiple markets. The results conclude with an evaluation of the given KPI to derive the final assessment of the substrate mixture optimization.

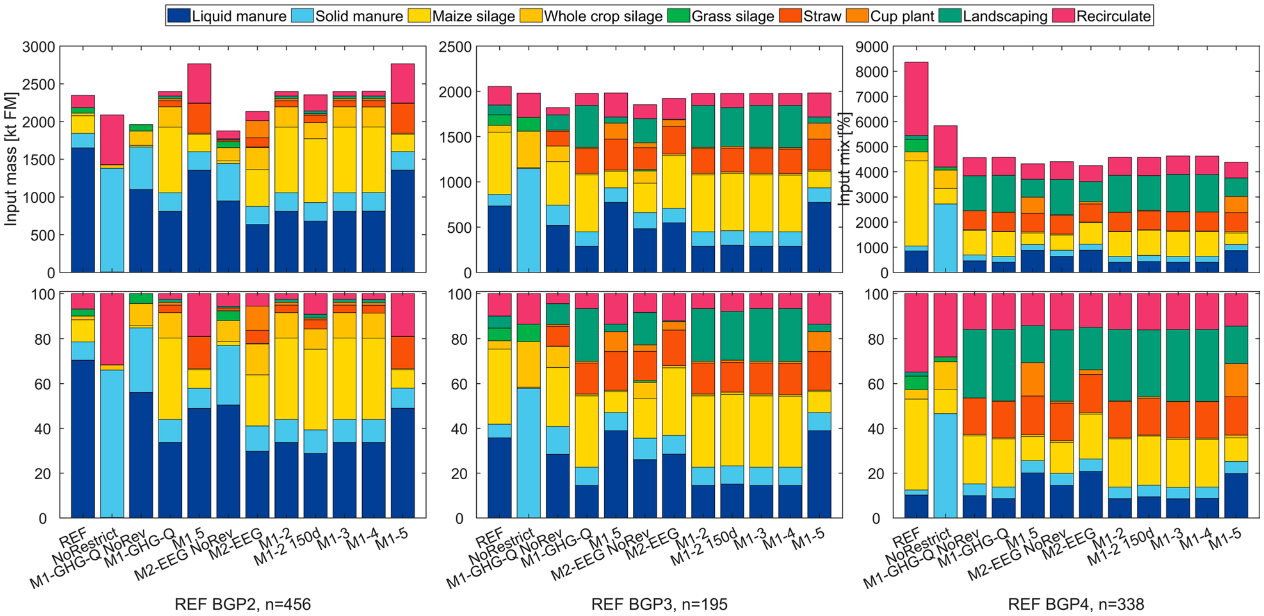

Fig. 3 Comparison of the absolute (top) and relative (bottom) optimal substrate mixture of the market variants for all BGPs in clusters REF BGP2–4

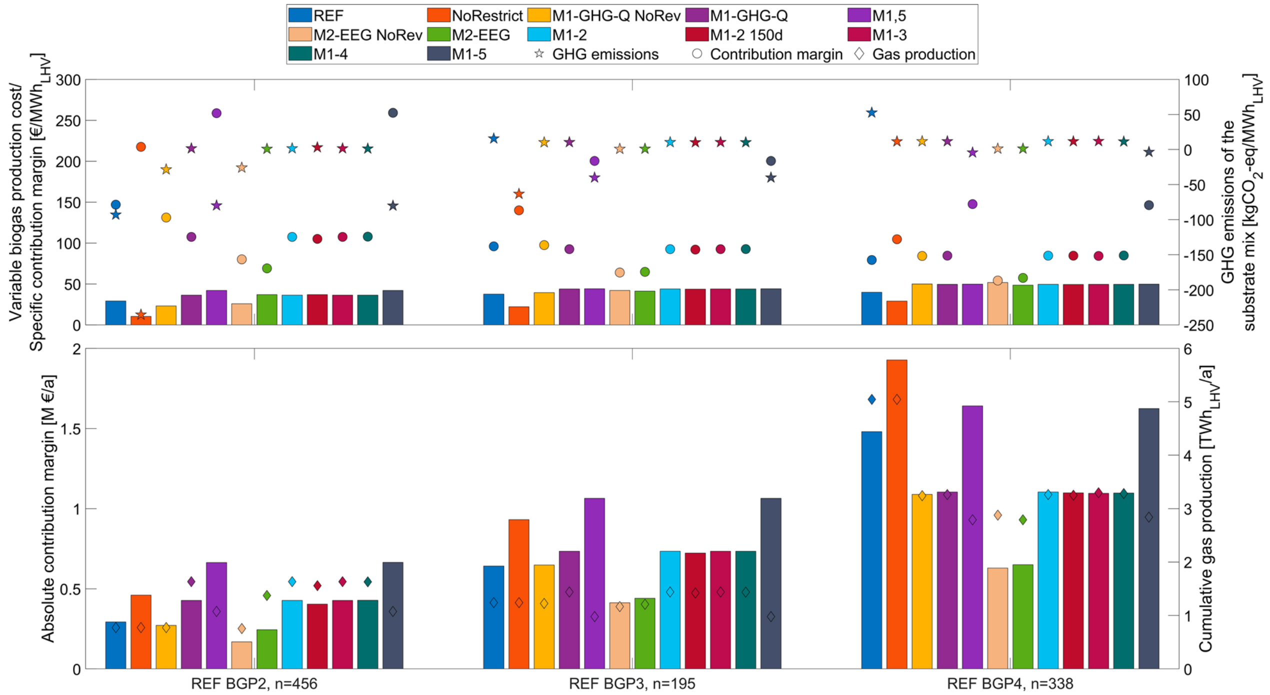

Fig. 4 Impact of the assessed setting variants for clusters REF BGP2–4 on variable biogas production cost, specific and absolute contribution margin, GHG emissions and cumulative gas production of all BGPs in the respective cluster; specific values are shown as weighted means (by weighted means)

Optimal substrate mixture

The optimal substrate mixture of the different market variants is shown in Fig. 3 for the clusters REF BGP2–4 as absolute sums across the cluster (top) and relative values (bottom). Results of clusters REF BPG 1 and 5 are shown in Figure 1 and of all BGPs in Figure 2 of the Additional file 3. In general, there is a strong effect of process constraints and substrate availability on the optimal substrate mixture (compare REF with NoRestrict). If substrate availability is not an issue (NoRestrict), solid manure would be the most valuable substrate for process restrictions and cost reduction (based on the underlying substrate properties).

Market constraints (Eqs. (8–10)) further restrict the optimal solution of the variable biogas costs. Impacts of constraints, such as the maize cap in M2-EEG, lead to less total input but more straw (M2-EEG NoRev). M1-GHG-Q NoRev usually leads to more maize silage and less manure. The difference between these two market constraints is less strong for the REF BGP4 cluster and highlights the great plant-specific differences. It is difficult to transfer the optimal substrate mixture, e.g., for M1,5, from one REF BGP to another. In addition, some BGPs, such as REF BGP4, are much more constrained in their production than others due to high reference shares of energy crops, low availability of manure and small potentials to increase gastight digester system. With additional market constraints, the substrate mixture becomes more diverse compared to REF, and the role of maize silage decreases.

Considering market revenues, the optimal substrate mixture between BGPs changes further. For example, the revenues of M1-GHG-Q lead to an intense usage of maize silage for REF BGP2 and landscaping material for REF BGP3. Market incentives like M1,5 can also mean using less manure is more optimal than the REF market variant for BGPs with high manure shares, such as REF BGP 1 and 2. In general, straw, landscaping material, and cup plant gain considerably due to the GHG reduction requirements and the consideration of revenues. Since M2-EEG revenues are not substrate specific and comparatively lower, there are fewer changes in the substrate mixture when considering revenues compared to M1-GHG-Q (compare M1-GHG-Q NoRev to M1-GHG-Q with M2-EEG NoRev to M2-EEG). Under very high market revenues, such as those of M5-Adv.GHG-Q, low GHG emission substrates are incited the most, leading to higher recirculation shares. Landscaping material is an exception, as it was not classified as a residues in this study and, therefore, not eligible for M5-Adv.GHG-Q. Manure also shows the highest shares for M5-Adv.GHG-Q compared to the other variants.

Table 5 Limiting constraints of the model variants in comparison to the boundary condition for REF BGP2; constraints limited by the boundary condition are marked in bold

Constraint	Boundary condition	Unit	No restrict	M1-GHG-Q NoRev	M1-GHG-QM1,5		M2-EEG NoRev	M2-EEG	M1–2	M1–2 150d	M1–3	M1–4	M1–5
Methane production	1751	MWh_{LHV}	**1751**	**1751**	4976	3871	**1751**	4374	4976	4976	4976	4976	3871
DSC	196	d	298	**196**	**196**	**196**	**196**	**196**	**196**	**196**	**196**	**196**	**196**
GHG emissions	8 (M1and5)/0 (M2and4)/1000 (M3-NG)	kg/MWh_{LHV}	−258	−34	8	−23	−34	0	**8**	**8**	8	**8**	−23
$TS_{In, digester}$	36%		19%	18%	29%	27%	18%	30%	29%	29%	29%	29%	27%
$TS_{Out, digester}$	15%		**15%**	13%	14%	**15%**	13%	**15%**	14%	14%	14%	14%	**15%**
OLR	6	kg VS/m^3 d	2.86	2.79	**6.00**	**6.00**	2.79	**6.00**	**6.00**	**6.00**	**6.00**	**6.00**	**6.00**
HRT digester	40	d	52	52	45	40	52	45	45	45	45	45	40
HRT gastight system	0 (M1/3/4/5)/150 (M2)	d	342	228	198	199	228	197	198	198	198	198	199
Maize cap	0 (M1/3/4/5)/35 (M2)		0%	0%	67%	34%	0%	**35%**	67%	67%	67%	67%	34%

Increases compared to REF are small, even though the availability was increased to 130% of REF. In absolute terms, manure usage does not increase even for M5-Adv. GHG-Q. The M1–2, M1–3, M1–4, and M1–5 changes are very small compared to M1-GHG-Q and M1,5 due to the comparatively low revenues of M2-EEG, M3-NG, and M4-GreenG.

Effects on variable biogas costs and GHG emissions

The plant-specific differences are also observed for the specific variable biogas costs, contribution margin, and GHG emissions for the clusters REF BPGs 2–4 in Fig. 4 (see Table 6 for the values and Figures 3 and 4 of the Additional file 3 for clusters REF BPG 1 and 5 and all BGPs). The contribution margins of market variants without revenues are based on hypothetical revenues in M1-GHG-Q. Since eligibility due to market constraints is not considered in these cases, contribution margins might be higher than market variants with revenues. It also should be noted that the difference between specific contribution margins can be small. A lower specific contribution margin may not necessarily mean a better result since production volumes and the capacity utilization of digesters also change. Hence, Fig. 4 also shows the absolute contribution margin (objective of the optimization) and biogas production volume at the bottom.

Even with strong market constraints, a cost reduction compared to REF is possible for some REF BGPs (1 and 2). Usually, though, there is an increase in variable biogas costs, which is often amplified by considering revenues. This increase goes along with an increase in biogas production (bottom of Fig. 4) if not limited by market constraints. At very high revenues for low GHG emission substrates such as manure, the optimal biogas production reduces again. In comparison, the highest contribution margins are achieved for all BGPs in M1,5, except for the hypothetical contribution margins of NoRestrict for REF BGP4.

Differences in specific costs and contribution margins between market variants are higher for BGPs with high manure shares, such as REF BGP1 and 2. With higher manure availability, these BGPs offer a larger solution space, are less limited by constraints, and have a greater potential to improve contribution margins and profitability. The previous difference in production (REF) between BGPs tends to even out due to market revenues. The range of production for different BGPs but also the ratio between production and digester and digestate storage volumes become closer. This also means digester and digestate storage volumes become more decisive.

In comparison, the effects on GHG emissions are very small because GHG reduction restrictions are not a limiting factor, especially in the case of M1-GHG-Q/M5-Adv. GHG-Q. However, the revenue incentives of M5-Adv. GHG-Q lead to lower GHG emissions. An exception is REF BGP2, which shows a slight increase.

Limiting constraints

Table 5 compares the values for the constraint parameters, based on the optimal solution, with corresponding boundary conditions of the individual REF BGP2. It is clearly shown that the methane production constraint is active when there are no revenues (NoRestrict, M1-GHG-Q/M2-EEG NoRev). It also means it is not a limiting factor since the production target can be met while respecting all other constraints. This is not always the case, as shown in Fig. 4 for cluster REF BGP4. For REF BGP2, the DSC is the most limiting constraint because the derived value, except for NoRestrict, is always at the boundary condition. The second most limiting constraint is the OLR, which is always limiting in the presence of revenues.

The percentages of BGPs in the REF BGP2 cluster that are limited by a constraint are shown in Table 6 to draw more general conclusions. Results for the other REF BGP clusters are in Tables 1–4 in Additional file 3. Across all clusters, constraints, and market variants, the DSC and TS_{Out} are the most limiting factors. As shown in Table 6, the latter is particularly limiting in the presence of M5-Adv.GHG-Q revenues (M1,5 and M1–5) due to high incentivization of straw. Further limiting constraints are the $HRT_{digester}$ and the OLR. The former is also strongly limiting in the presence of M5-Adv.GHG-Q. The OLR is limited only in the presence of revenues and mainly for clusters REF BGP 1 and 2, but not for REF BGP 4 and 5. On the other hand, TS_{in} can be a limiting constraint for the latter two clusters.

M2-EEG is generally more constrained due to stronger boundary conditions. The GRT is generally more limiting than the maize cap, and the $HRT_{gastight}$ is comparatively negligible. However, it can be a limiting factor if all markets require it, e.g., for REF BGP1 and partially for REF BGP2. A comparison of the clusters shows that more constraints limit cluster REF BGP 3, and clusters REF BGP 4/5 by the least.

Optimal market shares and gains in contribution margin

Table 7 gives an overview of the total market shares of energy production across all BGPs for the market variants with revenues. It also shows the gains in contribution margins compared to a benchmark market variant. When considering revenues (M1-GHG-Q/M2-EEG), the gains in contribution margins are significant (up to 21%) and affect all BGPs. They are stronger for REF BGP clusters 1–3 (see Table 5 in Additional file 3 for cluster-specific gains). However, the gains are strongly dependent on

Table 6 Percentage of BGPs in cluster REF BGP 2 (n=456) limited by constraints for each market variant

Constraint	NoRestrict	M1-GHG-Q NoRev	M1-GHG-Q	M1,5	M2-EEG NoRev	M2-EEG	M1-2	M1-2 150d	M1-3	M1-4	M1-5
Methane production*	100%	100%	0%	17%	100%	9%	0%	0%	0%	0%	17%
DSC	14%	80%	100%	100%	74%	78%	100%	87%	100%	100%	100%
GHG emissions (M1-GHG-Q)	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
GHG emissions (M2-EEG)	0%	0%	0%	0%	29%	88%	0%	0%	0%	0%	0%
$TS_{In, digester}$	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
$TS_{Out, digester}$	100%	0%	23%	97%	14%	34%	23%	31%	23%	23%	97%
OLR	0%	0%	89%	70%	0%	73%	89%	81%	89%	89%	67%
$HRT_{digester}$	9%	0%	15%	82%	0%	14%%	15%	16%	15%	19%	82%
$HRT_{gastight\ system\ (M1\text{-}GHG\text{-}Q)}$	0%	0%	0%	0%	0%	0%	0%	13%	0%	0%	0%
$HRT_{gastight\ system\ (M2\text{-}EEG}$)	0%	0%	0%	0%	13%	13%	0%	13%	0%	0%	0%
Maize cap (M2-EEG)	0%	0%	0%	0%	5%	61%	0%	5%	0%	0%	0%

* The percentage of BGPs with production below the REF variants is shown for market variants with revenues

Table 7 Overview of market shares and gains in contribution margins (abs.) in comparison to a benchmark for market variants with revenues

Market variant	M1-GHG-Q (%)	M2-EEG (%)	M3-NG (%)	M4-GreenG (%)	M5-Adv. GHG-Q (%)	Mean gain of BGPs with a gain (%)	Share of BGPs with a gain (%)	Total gains across all BGPs (%)	Benchmark
M1-GHG-Q	100.0	0.0	0.0	0.0	0.0	26	100	21.6	M1-GHG-Q Norev
M1,5	38.3	0.0	0.0	0.0	61.7	53	100	55.0	M1
M2-EEG	0.0	100.0	0.0	0.0	0.0	17	100	12.2	M2-EEG Norev
M1–2	100.0	0.0	0.0	0.0	0.0	0	0	0.0	M1
M1–2 150d	95.6	4.4	0.0	0.0	0.0	0	0	– 5.0	M1
M1–3	99.9	0.0	0.1	0.0	0.0	91	1	0.1	M1
M1–4	96.7	0.0	0.1	3.3	0.0	25	6	0.3	M1
M1–5	37.3	0.0	0.3	1.0	61.4	42	4	0.2	M1,5

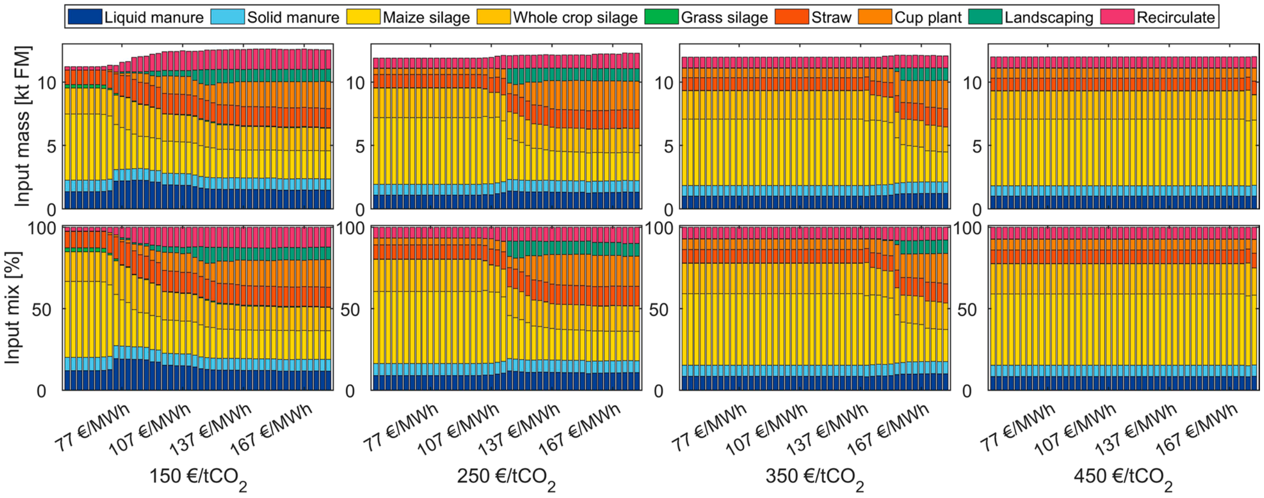

Fig. 5 Changes in substrate mixture for changing market prices in M2-EEG and different GHG quota prices levels (variant M1–2)

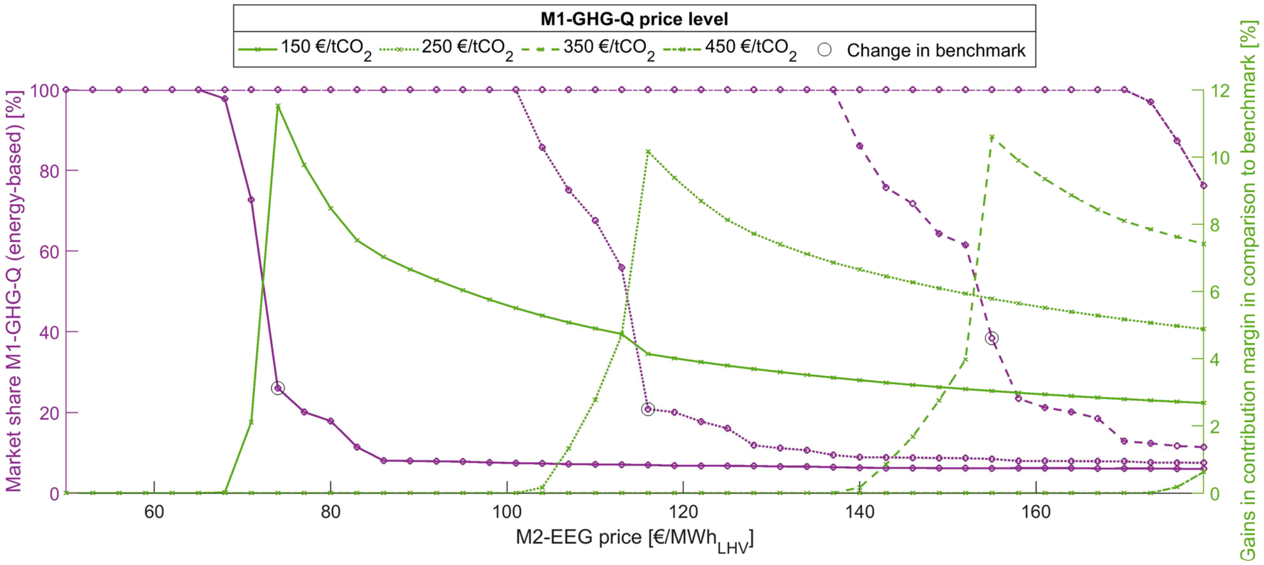

Fig. 6 Changes in market share of M1-GHG-Q (purple) and contribution margin gains (green) with respect to biomethane price in M2-EEG for different GHG quota price level (setting variant M1–2)

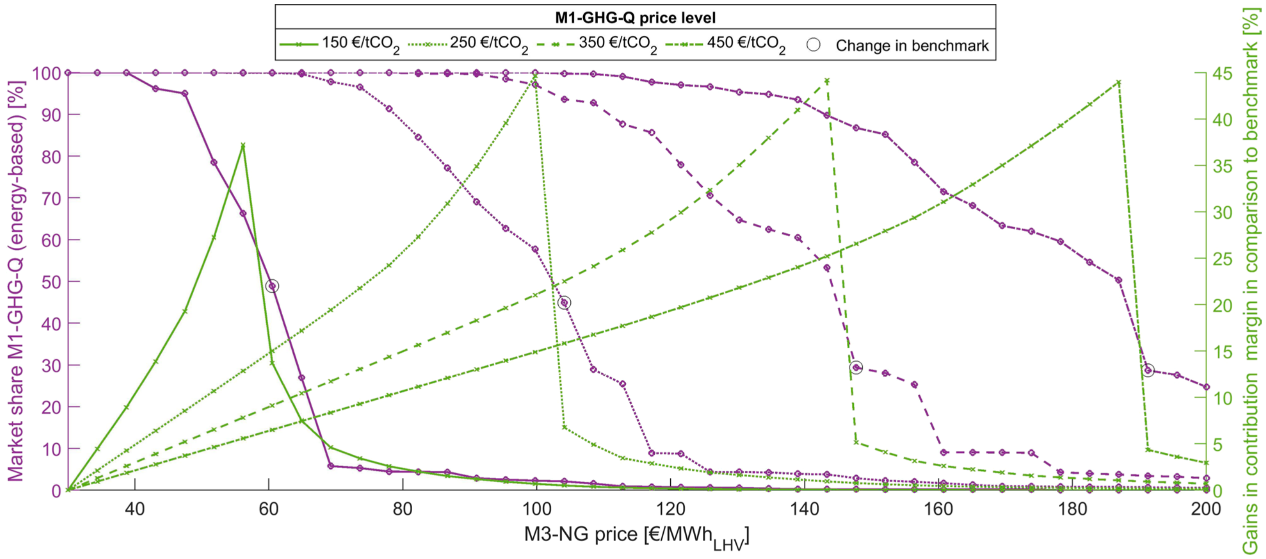

Fig. 7 Changes in market share of M1-GHG-Q (purple) and contribution margin gains (green) with respect to biomethane price in M3-NG for different GHG quota price level (setting variant M1,3)

the underlying market revenues, e.g., they are stronger for M1-GHG-Q than M2-EEG and even stronger for M1,5, since the revenue potential is higher. The higher revenues of M5-Adv.GHG-Q would also lead to a more even distribution of gains across the different REF BGP clusters.

When integrating multiple markets, market shares show that usually, a lead market attracts most of the biomethane volume. With the current incentive framework, this would be the transport fuel sector (M1-GHG-Q/M5-Adv.GHG-Q) which means that hardly any biomethane is available for other energy sectors (M2-EEG to M4-GreenG). This also leads to very small total gains (0.1 to 0.3%) in the optimization of multiple markets (M1–2 to M1–5) compared to the benchmarks of M1-GHG-Q or M1,5. M2-EEG does not matter in these market variants unless the $HRT_{min,\ gastight}$ constraint is applied to all markets. In practice, this can be the case, as the $HRT_{min,\ gastight}$ is often part of the permit for the whole BGP. The introduction of M3-NG affects very few BGPs, but strongly. These few BGPs are only found in the REF BGP clusters 4 and 5. The introduction of M4-GreenG affects slightly more BGPs (6%), with a mean increase of 25%. This effect is reduced when M5-Adv.GHG-Q is present (M1–5).

Sensitivity analysis

As shown by the dominance of M1-GHG-Q/M5-Adv.GHG-Q, market price levels are decisive. The sensitivity analysis, therefore, focuses on changes in these price levels. This includes not only the price ratio of different markets but also price levels in relation to changing market requirements and substrate costs. This also provides a more robust determination of potential contribution margin gains from optimizing multiple markets.

Price relation of M2-EEG and M1-GHG-Q

Figure 5 shows the effect of increasing M2-EEG revenues on the substrate mixture for four GHG quota price levels ranging from 150 to 450 €/tCO_2-eq. There is a clear market shift from M1-GHG-Q to M2-EEG for each price level highlighted by the “jump” in the substrate mixture, e.g. around 75 €/MWh at 150 €/tCO_2 (see Fig. 6 for comparison). Maize silage is mainly replaced by cup plant and, as prices increase, also by landscaping material. The use of manure also increases at the shift but decreases later at lower GHG quota price levels (150 €/tCO_2-eq). These changes in the substrate mixture are linked to a sharp drop in GHG emissions, which are roughly halved. They can be attributed to the higher GRT in M2-EEG (see Figure 7 in Additional File 3). These effects occur for each CO_2 price level but require higher and higher biomethane prices in M2-EEG.

As shown in Fig. 6, the price range for the market shift is very small but widens as the price level of the GHG quota increases. Within this range is a contribution margin optimization potential of around 10% (right *y*-axis). The potential gains depend strongly on the benchmark, which corresponds to the single market optimization of the leading market (shares > 50%). Figure 6 also illustrates the incentive asymmetry between the two markets. If the price level in M2-EEG is below the relevant price range, 100% of the biomethane will go to M1-GHG-Q.

Table 8 Overview of trends and conclusion taken from sensitivity parameters

Sensitivity parameter	Change in substrate mixture	Costs, contribution margin and emissions	Market shares and shifts	Figures in Additional file 3
Increases in energy crop prices lead to …	Maize silage and cup plant replaced straw and … • Landscaping (M1-GHG-Q NoRev) • Whole crop silage (M1-GHG-Q) manure (M1,5)	Slight increase in the specific contribution margin of (M1–5, M1,5) • GHG emissions reduce but only if revenues are present • Contribution margin (abs.) and production reduce strongly	Decrease in M1-GHG-Q share in favor of M5-Adv.GHG-Q and M4-GreenG (the ratio between the gaining markets is not developing linearly with higher EC prices)	Figures 10 and 11
Increases in non-energy crop prices lead to …	• M1-GHG-Q: less straw and cup plant in favor of landscaping • M1,5: less whole crop silage in favor of maize	• Slight increase in GHG emissions, a decrease in production (M1-GHG-Q, M1–2) and contribution margin, but much less strong compared to EC increases • Increase in production when M5-Adv.GHG-Q present (shift to M1-GHG-Q)	• M1-GHG-Q slightly gains shares in favor of M5-Adv. GHG-Q and M4-GreenG • Slight gains in contribution margin with M4-GreenG being present, i.e., M1–5 compared to M1,5	–
Increases in GRT M1-GHG-Q vs. M2-EEG prices lead to …	• Increases in manure and straw (M1-GHG-Q) in favor of maize/whole crop silage, landscaping andcup plant • Changes are not linear between 85 and 88% (strong market shifts)	• Strongly reduces GHG emissions, if M2-EEG is less valuable or there is no "escape market" (M1-GHG-Q) and production • Decreases in contribution margin • Increases in production if there is a strong market shift (M1–2 BM120)	Increases in GRT in M1 -GHG-Q shift market share to M2-EEG, the shift… • Depends on M2-EEG price level • Is small when market price differences are large and vice versa	Figures 12 and 13
Increases in GRT M1-GHG-Q vs. M3-NG prices lead to …		• Market shift towards M3-NG leads to higher production and GHG emissions • Reduction in contribution margin (abs.)	• Market shifts are less steep than M1–2 but occur earlier, i.e., does not require high M3-NG prices	–
Increases in GRT M2-EEG vs. M2-EEG prices lead to …	Increases in manure and straw in favor of cup plant, maize and whole crop silage (M2-EEG) • Strong substrate changes when a market shift occurs (e.g., BM160 between 72 and 75%)	• Strong production and GHG emission reduction (M2-EEG) • Change in production and emissions (increasing with higher M1 shares)	• Strongly increases M1-GHG-Q share, even for very high M2-EEG market prices	–
Increases in GRT M2-EEG vs. M1-GHG-Q quota prices lead to …	• Higher manure shares and less whole crop silage and cup plant	• Lower production, GHG emissions and contribution margin (abs.) until M1 gains considerable shares (> 30%)	• Lower M2-EEG shares (at low GHG quota levels)	Figures 14 and 15

Conversely, some biomethane always remains in M1-GHG-Q. As this share is higher with higher GHG quota levels, one reason is the very high substrate-specific value of substrate such as manure. The main reason, however, is the stricter restrictions of M2-EEG, such as the 150d of the gastight system and the maize cap. These reduce the maximum output in M2-EEG, while M1-GHG-Q allows evading restrictions with positive contribution margins and contributions to increase the total contribution margin.

Price relation M3-NG and M1-GHG-Q

Analogously, Fig. 7 shows that this asymmetric relationship is less strong, to the point that share of M1-GHG-Q converges to zero when there are no restrictions in the market with increasing prices (here M3-NG). This also causes the market shift to be less sharp, i.e., the price range of the market shift is larger. On the other hand, gains in contribution margins would be much higher, although this may be due to the chosen benchmark. Regarding the substrate mixture, higher M3-NG

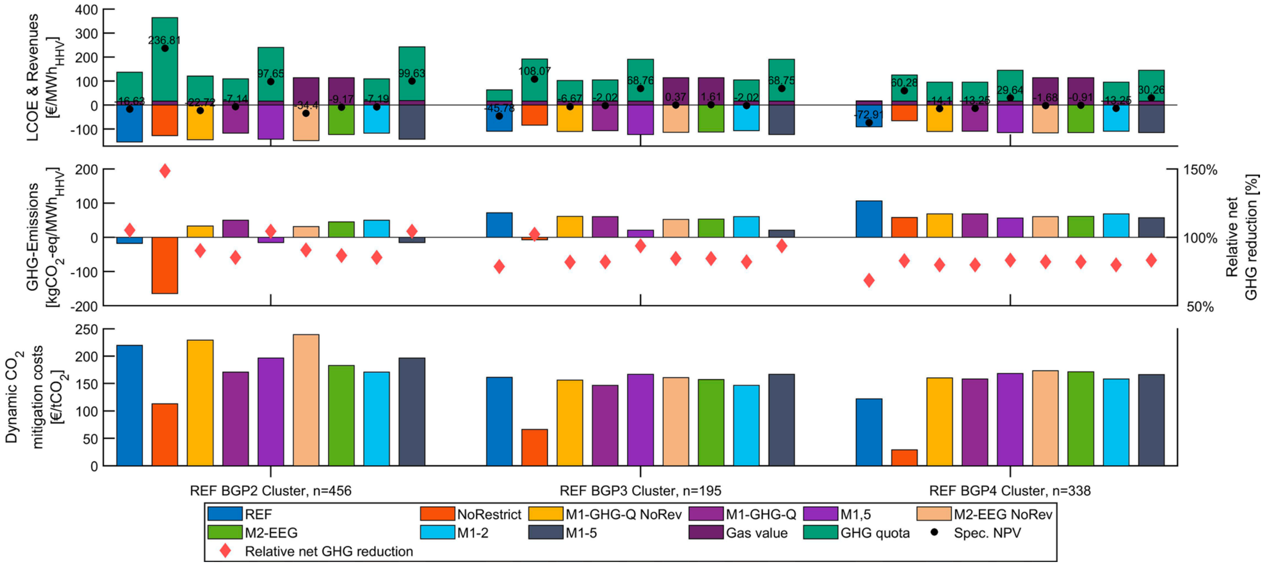

Fig. 8 Comparison of different model setting variants by selected KPIs for clusters REF BGP 2–4. The values were presented as weighted means over all BGPs in the respective cluster (considering each BGP gas production capacity as a weight)

shares lead to increases in the share of maize, grass, and whole plant silage while the share of manure and straw decreases (same for cup plant at higher GHG quota prices). Likewise, GHG emissions and gas production increase. The extent of the increases depends strongly on the underlying GHG price level, i.e., it is stronger at low GHG quota prices (see Figures 8 and 9 in Additional file 3 for details).

Further sensitivity parameters

All effects of the other parameters of the sensitivity analysis are given in Table 8. The corresponding Figures are given in Additional file 3. The results can be summarized as follows: when comparing two markets with different requirements and revenue structures, making one of these components in one market stricter or less valuable will shift market shares to another. Production and substrate mixture changes can then increase GHG emissions if the less stringent market becomes more economically attractive. This would contradict the original intent of tightening requirements. However, this dynamic is highly dependent on the underlying revenue relationship. Market shifts and further changes are unlikely under high GHG quota prices in M1-GHG-Q. Especially in the case of a market with basically no restrictions (M3-NG), tightening GHG requirements in the presence of high NG prices could lead to a "green market escape".

Energy crop (EC) price increases would favor markets such as M5-Adv.GHG-Q and lead to lower GHG emissions if revenues are present. Higher non-energy crops (Non-EC) prices would favor markets such as M1-GHG-Q and slightly higher GHG emissions. In general, higher substrate prices lead to lower production, although very high Non-EC prices reverse the tendency of lower production in M5-Adv.GHG-Q. Considering substrate-specific revenues becomes more critical when EC prices are high, i.e., the potential contribution margins for EC substrates gain compared to Non-EC. Vice-versa, it becomes less valuable when Non-EC prices are high.

Impact on key performance indicators

The results of the selected KPIs, such as NPV and CO_2 abatement costs, are shown in Fig. 8 as weighted means for the REF BGP clusters 2 to 4. The analog results for clusters REF BGP 1 and 5 are given in Figure 3 of the Additional file 3.

NoRestrict shows the best results for all KPIs and all REF BGPs due to its large solution space (no market restriction, full substrate availability). It can, therefore, serve as a maximum theoretical technical potential of a BGP. In comparison with REF, the addition of market constraints (M1-GHG-Q/2 NoRev) usually leads to larger increases in NPV (except REF BGP2), slight increases in CO_2 abatement costs (except REF BGP1 and 3) and decreases in GHG emissions (except REF BGP1 and 2). The reason is that restrictions such as GRT are more in line with the incentives of the GHG quota system. Adding revenues of M1-GHG-Q and M2-EEG increases NPV slightly further and decreases CO_2 abatement costs, while effects on GHG emissions are minimal. M1-GHG-Q and

M2-EEG usually do not lead to a profitable operation (except M1-GHG-Q for REF BGP1 and M2-EEG for REF BGP3). Comparing these two markets across all BGPs, M2-EEG offers better profitability despite higher LCOE and lower contribution margins in the optimization (see Figure 4 in additional file for all BGPs). The reasons are that the actual GHG quota revenues are lower or GRT requirements could not be met.[2] M2-EEG also leads to lower GHG emissions but slightly higher CO_2 abatement costs.

Contrary, profitability can be reached when considering the higher revenues of M5-Adv.GHG-Q. Only here, high contribution margins of gas production can cover fixed costs, such as investments in upgrading technology. Considering M5-Adv.GHG-Q also significantly decreases GHG emissions and increases net GHG reduction, which increases CO_2 abatement costs slightly. When comparing M1,5 with M1–5, the latter does not necessarily lead to a better outcome, as in the case of REF BGP1/2/3. Across all BGPs, there is a slight improvement, as the results of the market shares have shown. Only a small share of BGPs show an improvement when optimizing all markets.

Discussion

Potential gains in contribution margin, profitability, and other KPI

Integrating revenues and new restrictions into the substrate mixture optimization can increase contribution margins and profitability (NPV) compared to a cost-minimizing approach alone. Contribution margin gains range from 12 to 55%. Considering price changes, gains are slightly lower, ranging from 10% (M1–2) to 40% (M1,3). Setting the benchmark market is very decisive. The gains further increase by integrating multiple markets and optimizing them simultaneously. The additional gains are limited to a few BGPs. These are mainly found in REF BGP cluster which are more restricted such as REF BGP 4/5, while REF BPG 3 cluster is not affected at all.

These gains can be substantial, if strong restrictions in one market, e.g. M2-EEG, can be avoided by participating in another, e.g. M3-NG. The potential gains are smaller when the costs of strongly incentivized substrates (non-EC) and market restrictions are tight. Vice versa, revenue integration becomes more critical when EC prices are high and potential gains increase with less restrictive markets.

Similarly, to the effect of market restrictions, the potential gains by integrating market revenues are greater for BGPs with a larger solution space, such as REF BGP1/2. The revenue integration also leads to slightly higher LCOE, gas production, and GHG emissions while CO_2 abatement costs decrease. This contrasts with optimizing costs considering only market restrictions, which leads to lower LCOE, gas production, and GHG emissions but higher CO_2 abatement costs. The exception is the presence of M5-Adv.GHG-Q revenues, and to some extent M2-EEG, whose restrictions severely limit production.

Under M5-Adv.GHG-Q, gas production, and GHG emissions decrease considerably, but LCOE and CO_2 abatement costs increase again, as high GHG quota prices incentivize low yield and GHG emission substrates. Hence, current GHG quota prices are not optimal from a macroeconomic perspective but are also the only revenues that lead to a robust profitability case. Therefore, the normative double counting of the GHG emission reduction for advanced fuels (M5-Adv.GHG-Q) could be questioned.

Learn from and adapt to constraints

As the DSC and TS content in the digester outflow are the most limiting constraints across all markets and BGPs, investments in technologies such as additional storage volume or digestate separation should be investigated to ease constraints. The question remains whether the additional increase in contribution margin could pay for the new investments. Likewise, DSC requirements should not be increased, as it would reduce manure use in favor of whole crop and maize silage, thereby increasing GHG emissions. Other constraints are more plant/REF BGP cluster-specific. For example, the OLR is more relevant for smaller BGPs, and TS content in the input mix is more relevant for larger ones.

As the fuel market with its lower GRT is currently dominant, GRT is not a limiting constraint, nor does it affect GHG emissions. This changes when M2-EEG, with its higher GRT levels, is regarded individually. Unless there is a strong incentive for low GHG emission substrates (e.g., in M5-Adv.GHG-Q), uniform levels are required in all markets to have a noticeable reduction effect and prevent bypassing stricter GRT. Market-specific constraints, such as the maize cap, are also limiting, especially for smaller BGPs (REF BGP2/3/5). They are bypassed when other markets are an option. The effects of changing such market-specific constraints are relatively small, which calls into question their effectiveness in achieving goals such as reducing GHG emissions.

Drivers for market shifts

The leading biomethane market is the fuel market, which also has an asymmetric advantage due to its substrate-specific incentives and lower market requirements. However, our model approach may overestimate the substrate-specific revenues since on-site GHG emissions

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[2] Due to the additional GHG emissions in the Module 3 of the BGP-RepoMod.

such as the methane slip of the biogas production and biomethane upgrading lower the actual revenues of the GHG quota and are not considered in the optimization. Market shifts due to price changes are very sharp but level off at higher price levels or markets with fewer constraints (M3-NG). Changes in substrate costs or GRT also induce market shifts. For example, M5-Adv.GHG-Q gains shares from M1-GHG-Q at higher EC prices and vice versa for higher non-EC prices. Changes in GRT work similarly to higher price levels and level off the market shift gradients. However, heterogeneous GRT, e.g., higher GRT in the lead market and changes in GRT or prices, could lead to "market evasion" and higher GHG emissions. Hence, tightening requirements in markets with higher prices, e.g., higher GRT in M2-EEG, does not make sense if other less restrictive markets with sufficient price levels are an option. Market shifts also lead to strong changes in the substrate mixture, with corresponding effects on GHG emissions and gas production levels.

A critical review of the model approach and the solution robustness in the context of interdependencies and volatility

The presented model allows easy implementation of changes in market requirements and prices, substrate data (e.g., increasing costs of energy crops), or new markets for any BGPs. It has been shown that the optimal substrate mixture is very plant-specific and depends strongly on the framework conditions. This makes the optimization of the substrate mixture a suitable tool for finding quick and valuable solutions in operational use, e.g., to adapt to changing framework conditions or expected future developments. On the other hand, this makes transferability of the actual optimization results difficult and shortens the half-life of the validity. It is also difficult to generalize conclusions from specific markets of one BGP cluster to another. In reality, optimal substrate mixtures may vary even more, as results are highly dependent on the input data, such as plant-specific parameters and substrate data, which, with some exceptions, were assumed to be consistent across all BGPs. In addition, the optimal substrate mixture may be difficult to implement in practice due to further constraints on the biological process, local substrate availability, e.g., straw [50], and logistics.

In the BGP-RepoMod, the substrate mixture optimization is executed only once based on the averaged values of the time series for the expected future prices. In practice, prices for energy and substrates are subject to continuous volatility over the assessment period and interdependencies between model inputs and outputs. In addition, substrate provision, especially regarding energy crops, is usually planned long-term and may be less flexible, e.g., due to crop rotation.

In the case of market inputs, limited volumes in a single biomethane market, such as the transport fuel market, can lead to lower prices. The supply may significantly increase due to the significant potential of existing BGPs and biomethane upgrading plants. The latter predominantly supplied the biomethane CHP market and could switch to the fuel sector [51]. Hence, the assessed profitability of all BGPs may not be feasible on a case-by-case basis. On the other hand, not all BGPs will switch to biomethane upgrading simultaneously, and demand is expected to grow as GRT and gas-powered vehicles increase.

In the case of substrate cost inputs, the results show a clear trend toward higher straw use. Higher demand, which could be stimulated further by other sectors and applications, likely leads to price increases, as supply curves show for the south of Germany [52]. However, assumed straw prices are already high compared to these supply curves and other studies on the energetic use of straw [53].

Conclusions

Based on the sufficiently large BGP database used and the comprehensive sensitivity analysis, clear conclusions and general trends can be drawn from the present work. Integrating multiple markets' revenues and requirements makes significant gains in contribution margins and profitability possible. The level of gains depends strongly on the chosen benchmark market and the solution space size. The latter is constrained by the ratio of revenues and substrate costs, i.e., the substrate-specific contribution margins, and by the plant-specific characteristics in relation to the constraints. Substrate-specific contribution margins have a greater impact on the optimal substrate mixture and market shares.

For operators

As shown, unrestricted or a wide range of substrate availability is important in terms of costs and GHG emissions. The future substrate mixture will be more diversified than REF, with a strong reduction in maize silage and a strong increase in straw, cup plant, and landscaping material. The shares and ratio of these depend on specific-market incentives.

A goal should, therefore, be to make the BGP more robust and adaptable to a wide range of substrates through appropriate feeding and pre-treatment components, which is also relevant to TS limitations. The limiting constraint of the digestate storage capacity could be addressed by investing in more capacity or digestate treatment technology. The latter may also be helpful regarding TS limitations in the outflow.

More digester volume is key due to the lower calorific value of future substrates and the higher benefits of scale for capital-related costs. Higher gas production per volume does not necessarily correlate with higher profitability due to very high substrate-specific revenues (M5-Adv. GHG-Q) or strong market restrictions. Although, the latter does not always lead to an overall profitable outcome.

Likewise, high manure availability is an asset. Ideally, if solid manure is widely available and has the assumed properties, it would also be the best substrate for cost reduction. This would change the ratio between solid and liquid manure in favor of solid manure, equivalent to an indirect straw input.

Regarding sales and contract design, leaving sales volumes for short-term opportunities is recommended, especially when a market has low entry requirements (M3-NG) or potentially high future demand (M4-GreenG).

For climate policy

In terms of the regulatory framework, uniform requirements for biomethane markets are considered crucial for an effective climate policy. The focus should be on strong and targeted market entry thresholds like the GRT. However, the threshold should not be too high or increased too quickly, as higher GRT levels ($> -90\%$) could increase CO_2 abatement costs. Leaving solution space for energy crops or other regional options is crucial to increase plant-specific solution space. This is also because crop-related GHG emissions may decrease in the future due to decreasing background GHG emissions. The same policy demand is also made for the Danish case [17]. Hence, normative requirements such as the maize cap should be removed to allow a flexible substrate mixture solution for the wide heterogeneity of BGPs. Replacing maize silage with other energy crops also causes other negative effects due to its high area efficiency [54].

The normative GHG quota price setting in M5-Adv. GHG-Q causes similar negative effects on CO_2 abatement costs. Substrate-specific market prices, especially for manure, are an excellent way to develop the substrate mixture in the right direction as they reduce GHG emissions. Ideally, though, the value and price influence of the GHG reduction should be allocated to the sector in which it occurs. This means that the value of manure usage, which reduces GHG emissions in the agricultural sector, should be the same in each energy sector. There is no logical explanation for why such a reduction is more valuable in the transport sector than in others. An ideal long-term solution is carbon pricing in the agricultural sector. The remaining value in the energy sectors should only be determined by demand and supply mechanisms, e.g., by high sectoral reduction targets framed by strong and uniform GRTs.

The current regular GHG quota prices (M1-GHG-Q) or GRT (M2-EEG) are insufficient to increase general manure use. The future tightening of GRT will lead to a decrease in gas production from existing BGPs. Hence, there is a need for supportive policies to further incentivize the use of manure through the installation of additional digesters or new BGPs. Emphasis should be placed on facilitating investment in digesters and digestate storage, e.g., by investment support or simplified approval processes, as well as cooperative and logistical solutions.

Outlook for model developments

There are several ways to improve the substrate mixture optimization model for future use cases. Extending the time dimension in sub- or multi-year steps would allow for the incorporation of risk into the profitability assessment, particularly regarding price time series (futures) and changing GRTs. Integrating substrate cost functions that depend on the quantity used (non-linear or linear-approximated) could also create a more comprehensive model output. Furthermore, incorporating the impact of downstream GHG emissions into the model could improve the estimation of optimal market shares. Similarly, reducing normative substrate constraints and availability is important while adding new constraints, e.g., on nutrients. Integrating on-site CHP utilization as an additional market is essential for repowering concepts that combine biomethane upgrading with on-site CHP utilization. This also requires the integration of specific upgrading costs for all biomethane markets. Another focus could be on the portfolio optimization of biomethane volumes of existing upgrading plants by integrating other historical markets (existing biomethane CHP, different EEG versions). A portfolio optimization model could work for several BGPs in a portfolio by simplifying the model to a version without process restrictions.

Appendix

See Tables 9, 10, 11 and 12.

Table 9 Overview of current biomethane markets in Germany

Biomethane market	Transport sector/fuel	Heat (material use)	Power/CHP	Export
Market volume 2020 (GWh_{HHV})	1000	642	8435	233
Drivers/revenue sources besides natural gas price	GHG quota	Willingness to pay and RE heat obligations (low temperature). CO_2 prices, H_2 unavailability, decarbonization targets and green carbon demand (Industrial customers/process heat))	Electricity and heat price levels, EEG rates, flexibility value, voluntary commitments by utilities, higher heat utilization, and efficiencies of central power plants	CO_2 pricing, green gas quota (e.g., Switzerland), exemption from energy taxes
Framework regulation (GER)	REDII, BImschV, BEHG	GEG, BEHG	EEG, KWKG	ERGaR, country-specific regulations
Current opportunities besides high gas prices	LNG market ramp-up (development of central infrastructure and truck fleet), toll exemption, good availability of technologies (e.g., trucks)		Efforts to achieve independence, diversification, and long-term hedging of natural gas	Exchange between countries increasingly facilitated, demand and supply increases EU-wide + new EU targets (RepowerEU)
Challenges/uncertainties	high natural gas prices; Development of CNG market rather unclear; Further development of CO_2 pricing (e.g., ETS2), REDIII	Further development of CO_2 pricing (e.g., ETS2), REDIII	Further incentivization of green gases and seasonal storage, REDIII	Further development of CO_2 pricing (e.g., ETS2), REDIII

Table 10 Description of the setting variants of the substrate mixture optimization model

Model setting variant	Conditions
NoRestrict	• Unlimited bounds for all substrates (unlimited substrate availability for manure) • No regulatory or normative constraints • Setting a minimum level for the methane production
M1-GHG-Q NoRev	• Considering all relevant restrictions, excluding revenues • Setting a minimum level for the methane production
M1,5	• Considering both markets 1 and 5, including all relevant constraints and revenues
M2-EEG NoRev	• Considering all relevant restrictions, excluding revenues • Setting a minimum level for the methane production
M1–2	• Considering both markets 1 and 2, including all relevant constraints and revenues
M1–2 150d	• The same as M1–2 while considering the constraint of 150d HRT$_{\text{gastight system}}$ for both markets
M1,3	• Considering markets 1 and 3, including all relevant constraints and revenues
M1–3	• Considering markets 1 to 3, including all relevant constraints and revenues
M1–4	• Considering markets 1 to 4, including all relevant constraints and revenues
M1–5	• Considering all five markets, including all relevant constraints and revenues

Table 11 Characteristic plant parameters and their determined classes for the applied database to categorize representative reference BGPs

Parameter/unit	Rated power output (kW$_{el}$)			Substrate mixture (manure share) (%)			Digester volume (m^3)		
	Mean	Lower limit	Upper limit	Mean	Lower limit	Upper limit	Mean	Lower limit	Upper limit
Class									
1	623	400	–	76	51	100	4180	2629	–
2	284	202	400	43	28	51	1836	1220	2629
3	111	0	202	17	0	28	717	0	1220
Base	EEG data			EEG + regional data (M1 output)			EEG + regional data (M2 output)		

Table 12 Time series for gas prices and GHG reduction goals

Parameter	Unit	Static value[a]	2020	2025	2030	2035	2040	2045	Sources
GHG quota	€/tCO$_2$-eq	350	300	317	333	350	367	383	[36, 55, 56]
Natural gas	€/MWh	60	20	55	32.5	32.5	32.5	32.5	[20, 32, 57–61]
Green gas	€/MWh	150	150	142.5	130	115	100	80	[29, 60, 62–64]
GHG reduction target in the transport sector	%	0.65	0.67	0.69	0.78	0.78	0.78	0.78	[49, 65]
GHG reduction target in the electricity sector	%	0.70	0.70	0.70	0.80	0.80	0.80	0.80	[49]

[a] For sensitivity analysis

Abbreviations

BGP	Biogas plant
CHP	Combined heat and power
CNG	Compressed natural gas
DSC	Digestate storage capacity
EC	Energy crops
EEG	Renewable energy act (German: Erneuerbaren Energien Gesetz)
FM	Fresh mass
GG	Green gas for heat usage
GHG	Greenhouse gas
GRT	GHG emission reduction target
HHV	Higher heating value
HRT	Hydraulic retention time
KPI	Key performance indicators
LCOE	Levelized cost of energy
LHV	Lower heating value
LNG	Liquified natural gas
M1-GHG-Q	Market one—fuel market
M2-EEG	Market two—CHP market (EEG)
M3-NG	Market three—natural gas market
M4-GreenG	Market four—green gas market
M5-Adv.GHG-Q	Market five—advanced fuel market
NG	Natural gas
Non-EC	Non-energy crops
NPV	Net present value
OLR	Organic loading rate
RED II	Renewable energy directive II of the EU
REF BGP	Reference biogas plants
TS	Total solids
VS	Volatile solids

Supplementary Information

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Supplementary Material 1.

Supplementary Material 2.

Supplementary Material 3.

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Author contributions
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Availability of data and materials
Besides the core data provided in the main script and supplementary information, all datasets used and/or analyzed during the current study are available from the corresponding author upon reasonable request.

Declarations

Ethics approval and consent to participate
Not applicable.

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The authors declare that they have no competing interests.

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