

ORIGINAL RESEARCH

Processing Miscanthus to high-value chemicals: A techno-economic analysis based on process simulation

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Abstract

Thermochemical biorefineries for the production of chemicals and materials can play an important role in the bioeconomy. However, their economic viability is often questioned under the premise of the economy of scale. This paper presents a regional, modular biorefinery concept for the production of the platform chemicals hydroxymethylfurfural (HMF), furfural and phenols from the lignocellulosic perennial miscanthus, which can be cultivated on marginal and degraded areas. The paper focuses on the question of the minimum selling price of HMF and the optimal plant size for this purpose, using the region of Baden-Württemberg, Germany, as an example. Based on small pilot plant results, a scalable process simulation was created via AspenPlus. This allows different scenarios and process combinations of this multi-output biorefinery concept to be compared with each other. Using this, a minimum sales price for the main product HMF is calculated using methods of dynamic investment cost calculation according to the net present value method. Based on this, the plant capacity was scaled. The scenarios and sensitivity analyses show that, with an accuracy of $\pm 15\%$, regional biorefineries could already offer platform chemicals at prices of 2.21–2.90 EUR/kg HMF at the current stage of development. This corresponds to three to four times the price of today's comparative fossil base chemicals and is thus a competitive option from the authors' point of view. The local biomass and the heat prices were identified as the main influencing factors. As a result, the selection of the location will have a decisive influence on the economic viability of such concepts in the case of further development and optimization of the process in first demonstration plants.

KEYWORDS

agro-industrial biorefinery, furfural, HMF, hydrothermal processes, minimum production costs, platform chemicals, process optimization, regional bioeconomy, small-scale biorefineries, TEA

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1 | INTRODUCTION

To fight climate change and the depletion of non-renewable resources as well as the resulting challenges, some nations are pushing for a transformation process from a fossil-based economy toward a circular bioeconomy (Teitelbaum et al., 2020). The versatility of biological resources allows different utilization paths. Next to energy production, a wide range of biobased material utilization pathways exist, which shall be prioritized due to the cascade utilization hierarchy. According to the German Chemical Industry Association, about 18 million tons of fossil raw materials were consumed in Germany in 2017 as the raw material basis for organic chemistry. This corresponds to about 5% of fossil resource consumption in Germany that must be substituted with renewable resources in the chemical industry (VCI, 2020). After atmospheric CO₂, biomass-carbohydrates are the second largest renewable and sustainable carbon source on earth (Questell-Santiago et al., 2018), while carbon is needed to build up nearly every single chemical in usage. The target to avoid further consumption of fossil resources and instead to manufacture all chemicals, materials (and energy) in a sustainable and renewable way, cannot be reached by simply increasing the cultivation of plants. The worldwide and EU-wide available arable land per head is annually declining by 10% (The World Bank, 2016). This decline can even be more drastic due to extensive settlement areas, erosion, the effects of climate change and unsustainable use of land. Using the so-called first-generation biomasses such as sugars from corn, sugar beets or cereal grains, not only consumes arable land, but also competes with food production. This limits the socio-political acceptance of the bioeconomy due to the “food or fuel” debate. Therefore, alternative plant-based feedstock like lignocellulosic and the so-called second-generation biomass should be considered additionally.

Miscanthus as a high-yielding and low-input crop has been generating a lot of attention for years (Weijde et al., 2017). As a perennial C₄ crop, miscanthus conserves biodiversity and can be cultivated on marginal land (Clifton-Brown et al., 2017). This could minimize land-use competition with food and feed production (Clifton-Brown et al., 2017; Valentine et al., 2012). Its cultivation contributes to soil health and fertility and can reduce soil erosion (Winkler et al., 2020). Moreover, miscanthus binds carbon in the soil, primarily through rhizome growth, and thus often performs better in life cycle analyses than other traditional energy crops like maize (Kiesel et al., 2017). This low environmental impact is a strong argument for feedstock use in biorefineries by leading to end-product emission reductions. In addition to this article, which focuses on the process design and cost estimation of a miscanthus

biorefinery, another article is currently in progress which compares the environmental impacts of the miscanthus biorefinery with a fructose-based biorefinery.

Currently, miscanthus is mainly used as an energy crop. In addition to its use as a fuel, processes for gasification, pyrolysis or bioethanol production are also being strongly discussed and, in some cases, have already been developed to industrial maturity (cf. Bomgardner, 2019; Lask et al., 2019). Yet, the material use of miscanthus brings also great potential. In addition to the production of biofuels (Lee & Kuan, 2015), bioenergy and building materials (Uihlein et al., 2008), the miscanthus components cellulose, hemicellulose and lignin are suitable for the production of platform chemicals such as 5-Hydroxymethylfurfural (HMF) and furfural as well as chemicals from phenolic mixtures (Dahmen et al., 2019; Świątek et al., 2020). Miscanthus can become a major source of biomass in future agro-industrial or rather ligno-industrial value chains by emphasizing lignocellulosic biomass.

The possibilities for HMF applications are broad. That is one of the reasons why HMF is listed in the US department of energy top 14 list of the most promising biobased platform chemicals for the future (Bozell & Petersen, 2010). For example, it has an enormous potential to replace the human toxic, volatile formaldehyde. HMF can also be the starting point for fungicides or as part of electron transfer catalyzers. Moreover, fuels and fuel additives and food additives are made of HMF (Krawielitzki & Kläusli, 2015). HMF is also a biobased chemical building block for the production of polyesters, polyamides and other plastics (Dutta et al., 2012).

Furfural is another biobased platform chemical and an important furan derivative for the future biobased chemistry (Bozell & Petersen, 2010). It is produced from hemicellulose and can also substitute formaldehyde. One of the main applications of furfural is hydrogenation to furfuryl alcohol. The annual production of furfural ranges between 300 and 700 kt (Schwidorski & Kruse, 2016). Other applications include preservatives via furandicarboxylic acid (Ghosh et al., 1982) and furan resins as well as additives for resin production via the mentioned furfuryl alcohol (Gandini & Belgacem, 1997).

The phenolic mixture which mainly contains phenol, catechol, eugenol, etc. from the lignin fraction of miscanthus also offers potentials, especially in the pharmaceutical industry for drug synthesis (Barboza et al., 2018; Pramoda et al., 2010) or as an insecticide (Huang et al., 2002).

This wide range of applications led to the development of the miscanthus multi-output biorefinery concept presented in this research paper. A broad range of conversion options for the material use of lignocelluloses such as miscanthus is known and illustrated in Supplementary Materials S1. In addition to thermochemical processes as

analyzed in this research, the biomass can also be refined into valuable materials by biotechnological or physical processes. With the help of such biorefinery concepts, the raw material transition in the chemical industry can be accelerated. Hence, the aim of the research is to develop and evaluate a multi-output lignocellulose biorefinery concept for the regional valorization of miscanthus via hydrothermal processing into platform chemicals.

1.1 | Research approach

The multi-output miscanthus biorefinery produces the chemicals HMF, furfural and a monomeric phenolic mixture as well as the by-products heat and carbonisates. The five processing modules with its submodules produce the chemicals, a biogas plant, which is outside the system boundaries, provide the necessary infrastructure as illustrated in Figure 1. In all cases, A represents the synthesis or reaction and B the separation unit.

1. Miscanthus pre-treatment (M 1)
2. Furfural production (M 2)
 - a. Furfural synthesis (M 2A)
 - b. Furfural separation (M 2B)

3. HMF production (M 3)
 - a. HMF synthesis (M 3A)
 - b. HMF separation (M 3B)
4. Phenol production (M 4)
 - a. Lignin depolymerization (M 4A)
 - b. Separation of the phenolic compounds (M 4B)
5. Biogas plant for waste stream treatment, nutrients regeneration and energy provision (M 5)

All of the processes used to produce the desired chemicals can be grouped under the term hydrothermal processes (HTP) in acidic and aqueous media. According to Davidson (Davidson et al., 2021), these are preferable to the alternative solvent-based reaction media because of the lower environmental impact and better cost-effectiveness. In the pretreatment module M 1, the chopped miscanthus straw is decomposed with water and sulfuric acid in a hydrothermal process at about 200°C into its solid lignin fraction and a carbohydrate-rich solution consisting mainly of glucose, glucooligosaccharides and xyloses (Świątek et al., 2020).

The xylose dissolved in the process water is then converted to furfural in a hydrothermal process at 200°C and 20 min reaction time (furfural synthesis M 2A). The furfural is purified by a combination of a distillation and

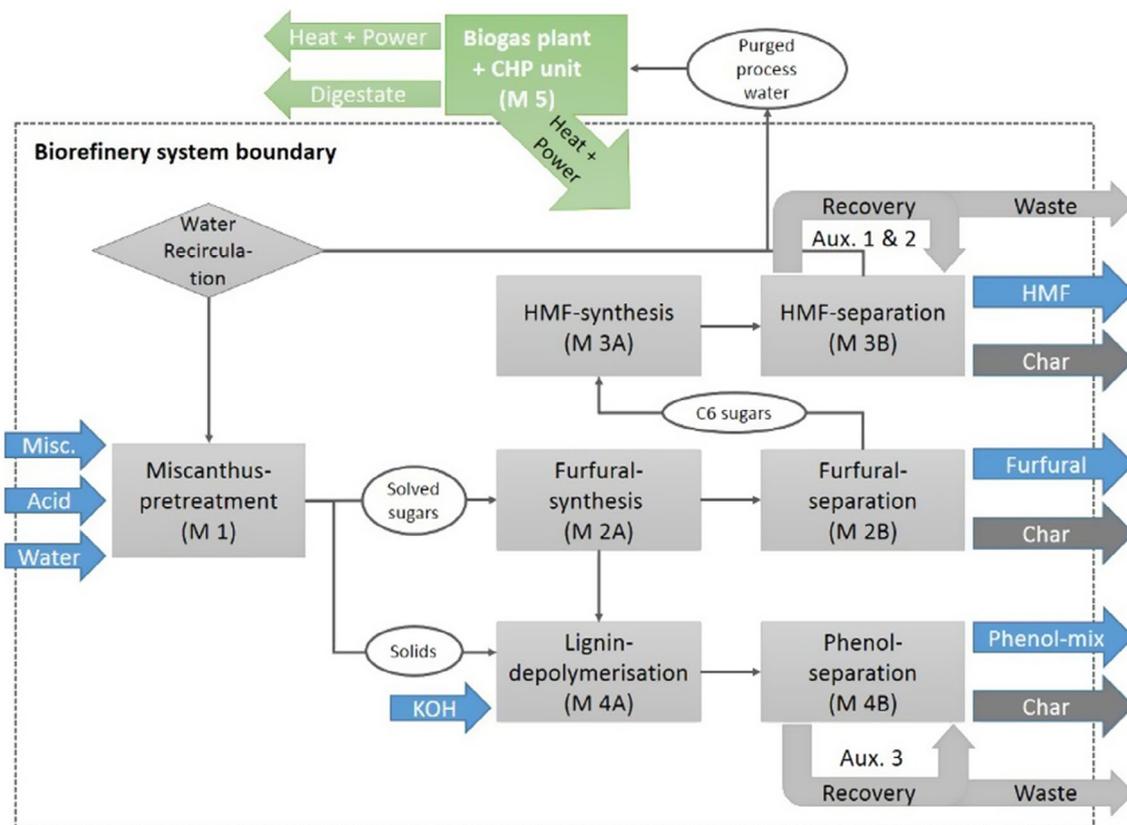


FIGURE 1 System boundary of the multi-product biorefinery with the processing modules (M1–M5). A, synthesis unit, B, Separation unit

a decanter in the separation module M 2B into a liquid product. As with any hydrothermal process, a carbonaceous product is formed in the synthesis unit M 2A, which is discharged from the system as a byproduct in the separation unit (M 2B), as seen in the Sankey diagram in Figure 3. Meanwhile, the dissolved glucose in the bottom of the distillation continues to react only to a small extent is further processed in the reactor of the HMF module at 210°C for 18 min to form HMF and carbonisates. The approximately 0.5 wt.%–1 wt.% HMF solution is refined to a degree of purity between 80 wt.% and 90 wt.% in a separation unit. This requires auxiliary materials, most of which can be reused. However, little part of these substances must be replaced to avoid, for example, the accumulation of impurities in the auxiliaries. Due to an ongoing patent application (patent number EP 21152776.7), the HMF separation (M 3B) cannot be described in detail. The products are the purified HMF and an acidic, aqueous process water stream containing mainly unreacted glucose and other byproducts such as short-chain organic acids or aldehydes (Wüst et al., 2020). This stream is used in M 1 to mix the fresh miscanthus, which has a water content of approx. 10 wt.%. This feedback stream increases the overall HMF yield and reduces the demand for fresh water and acid. However, to prevent the byproducts and, for example, salts from accumulating too much, a small part of the process water is discharged from the biorefinery system via the biogas plant, as described before. Via the digestate, the nutrients are returned to the fields in the sense of a sustainable circular economy, and the renewable energy generated in the biogas plant is partly used for the lignocellulosic biorefinery.

In module M 4A, the lignin depolymerization reactor, the lignin slurry is decomposed with KOH at 360°C and

corresponding saturation vapor pressure to form a phenolic mixture consisting of monomeric substances such as catechol and phenol and a number of other phenolic and oligomeric compounds. In the process, solid carbonisates are again formed. The focus on the lignin use within this work was to generate monomeric aromats for further conversion to adipic acid and antioxidants. Therefore, all other products have been lumped into one product stream containing oligomeric and polymeric substances derived from the lignin (see Figure 3). The process is not yet fully developed and improvements are expected in terms of conversion yields and valorization of the product fraction.

The process water is mixed in the separation module M 4B with ethyl acetate as extraction solvent. This is finally evaporated and circulated. As in the HMF separation unit (M 3B), a small portion of the solvent is disposed and replaced with fresh agent to minimize the accumulation of water and impurities in the system (unpublished results, c.f. acknowledgements).

An existing biogas plant (M 5) is assumed at the location. The biogas plant is not within the system boundaries of this study, among others because techno-economic assessments of biogas plants are already accessible (Shafiei et al., 2018). For the material and energetic coupling of biorefineries and biogas plants, a separate research project started at the University of Hohenheim at the end of 2020. The furfural and HMF modules M 2 and M 3 have a technology readiness level (TRL) between 5 and 6 and are located at an agricultural research facility of the University of Hohenheim (Foto of the facility in Supplementary Materials S1). The lignin processing module M 4 has a lower technology readiness level of 4.

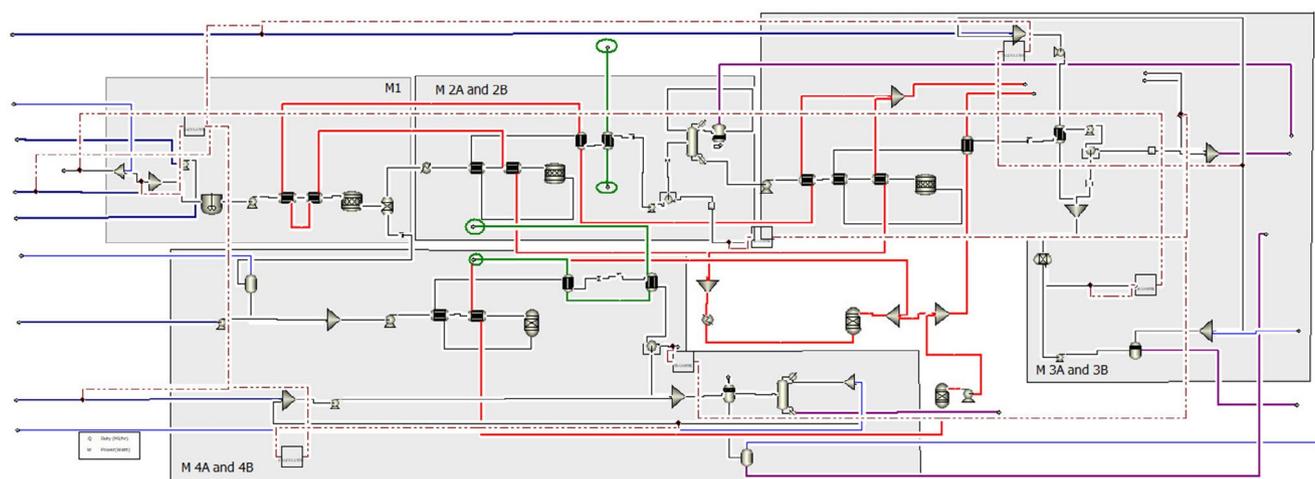


FIGURE 2 Main flowsheet of the miscanthus biorefinery. Purple, products; red, heating energy; green, cooling energy; dark blue, auxiliaries; light blue, purge or waste streams. M1 to M 4, modules of the biorefinery

2 | MATERIALS AND METHODS

2.1 | Process simulation

The data on the mass and energy flows as well as on the dimensions of the main apparatuses originate from an AspenPlus process simulation (V.9 & V.11). The method used in this simulation is NRTL. MIXCISLD is used as simulation stream class. Thus, mixed conventionals and conventional solids, but no nonconventional solids and no particle size distribution are taken into account. The reactions along the process chain are described with stoichiometric reactors (RSTOIC). The heat cycle is simulated by yield reactors and mainly heat exchangers to have an idea about the size of the heat exchanger surface area. These areas are also used for the TEA calculations. The separation operations are simulated with RADFRAC and FILTER blocks. The separation operations in M 3 (HMF module) are simulated with SEPARATOR blocks to protect details. Furthermore, calculator blocks are used to be able to simulate the input adjustments after recycling of the process water and auxiliary materials. Compared to small pilot plant trials, a process simulation enables large mass and energy flows to be mapped and optimization steps to be integrated by heat management including the size of heat exchangers, material flow management and recycling flows. This provides scale-up information at a very early stage of development. Since simulations can only represent reality to a limited extent, some processing assumptions were made:

- Complete conversion of hemicellulose to xylose.
- Solids were simulated as conventional solids of the respective platform chemical without side reactions.
- Carbon materials are discharged at a moisture content of 57 wt.% without additional drying.
- To avoid concentration of impurities, 2 wt.% of the solvent in module M 3B is hourly replaced with virgin material.
- The lignin is passed through the simulation as an inert substance until the phenol synthesis in M 4A.
- Moisture loss due to the temperature difference between the warm moist product stream from M 1 and the ambient temperature until further processing is simulated in M 4A to dewater the lignin slurry.
- Catechol, phenol, syringol and 4-methylcatechol are the key components for simulating the monomeric phenolic mixture—other compounds are neglected.
- Oligomeric and polymeric products, along with the resulting carbonisates, is defined as CHAR and is discharged as a solid and not recycled.
- 7 wt.% of the solvent ethyl acetate is not recycled and discharged due to possible impurities.

- All input material streams of the simulation have a temperature of 11°C, which is the rounded annual mean temperature in Germany in 2020 (Bundesamt, 2021).
- A temperature of 55°C is assumed as the flow back temperature of the heat transfer medium to the biogas combined heat and power plant (CHP).
- Due to the additional HEATER blocks inserted, heat losses are simulated at several points. In general, AspenPlus calculates material flows as adiabatic systems. In the heat transfer medium, the loss is assumed to be 5% and in the product stream 15% over the complete biorefinery process chain.
- Initially, hydrothermal, subcritical water is assumed as the heat transfer medium instead of low-temperature steam to be able to calculate with uniform physical models throughout the simulation.
- Pumps have a pump efficiency of 80%.
- To provide conservative data for the techno-economic analysis, all simulation results, including the heat exchanger areas, are rounded up to whole numbers.

The miscanthus biorefinery is divided into four process steps: module M 1, modules M 2A and 2B, modules M 3A and 3B, and modules M 4A and 4B as highlighted in gray in the process flowsheet in Figure 2 as well as two additional auxiliary material cycles (a heating cycle as highlighted in red, and a cooling cycle as highlighted in green). The purple mass flows in the right margin of the figure signal the product flows of the products furfural, HMF, carbonisates and phenolic mixture, which was split into two partial flows in the process simulation. The feedstocks miscanthus, fresh water, catalysts and auxiliary materials for the separation operations are marked in dark blue. Light blue are waste and residual streams. These include the removal of portions of contaminated auxiliary materials or the recycling streams.

2.2 | TEA assumptions

In the following, a techno-economic feasibility study of producing platform chemicals (i.e., HMF, furfural and phenol) from miscanthus provides insights into the economic demonstration of small-scale biorefineries at the example of the German state of Baden-Württemberg. The basis of the techno-economic analysis (TEA) is the process simulation, the small-scale pilot plant and the underlying experimental data explained and presented in the previous sections. The mass and energy balances of the process simulation provided the framework for the design of the apparatuses. Investment estimation methods were applied to map the pilot scale to industrial scale by applying a parametric model resulting in

a class three estimate, with a maximal accuracy range of -15% to $+15\%$, for the economic concept assessment (Christensen et al., 2005).

The detailed factors method was used to analyze the economic profitability of the proposed small-scale, modular biorefinery. The method estimates the capital expenditures (CAPEX) as investments for physical facilities and operational expenditures (OPEX) as operating costs as percentages of the total equipment costs and revenues. The construction costs are calculated as a percentage of the total equipment cost and a brownfield approach has been chosen. Prices are updated with current indexes to the reference year 2020. Due to the use of acids in the process, the standard construction material is stainless steel 316L.

The biorefinery concept is scaled from Scale 1, an on-farm concept with 500 kg, and ranging to Scale 10, a regional concept with 5000 kg miscanthus input per hour. The selection of apparatuses and the scaling factors are obtained from Peters et al. (2003), Chauvel et al. (2003) as well as Couper et al. (2005) and Turton et al. (2018). Scale 1 represents a small-scale biorefinery that can be operated by one or a few farmers in collaboration. In contrast, Scale 10 can be operated centrally by several farmers in a cooperative network. Both scales thus define the minimum and maximum theoretical capacity of the investigated biorefinery concept.

The TEA assumptions are summarized in Table 1 and cover the techno-economic profitability factors as well as further cost factors in accordance with a solid–fluid processing facility. In the following, the TEA figures are used for estimating the costs.

3 | RESULTS AND DISCUSSION

3.1 | Mass flow results used as raw data for the TEA

The Sankey diagram in Figure 3 shows an overview of the mass flow of miscanthus components through the biorefinery as a result of the process simulation. For simplicity and clarity, miscanthus is shown dry based and ash free and consists only of the components hemicellulose, cellulose and lignin. The mass flow is normalized to one ton. The descriptions of the different modules (process steps) are based in Figure 1. The Sankey diagram does not show the water consumed in the hydrolysis reactions during biomass decomposition but the water produced in the dehydration reactions (e.g., Furfural and HMF synthesis). Accordingly, in contrast to Figure 4, the Sankey diagram shows pure products without, for example, residues of solvents.

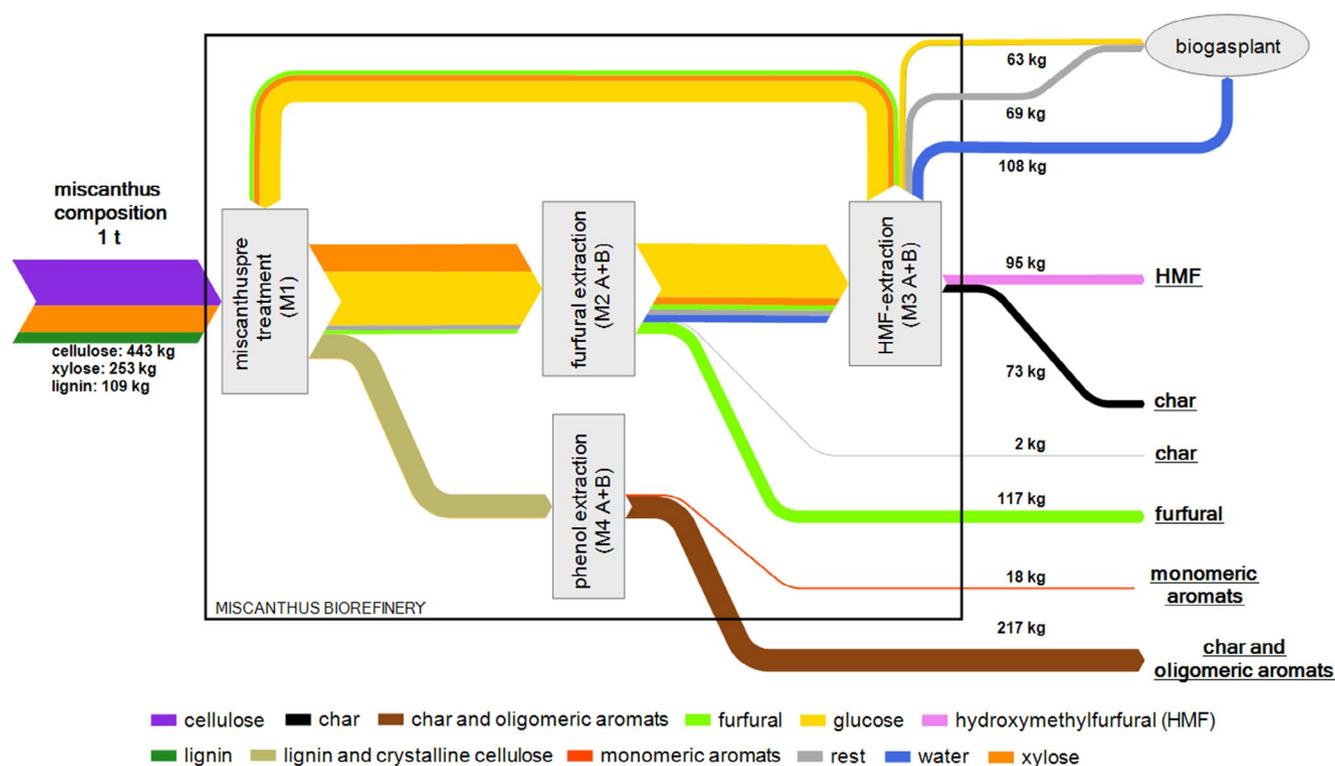


FIGURE 3 Sankey-Mass-Flow-Diagram of the miscanthus biorefinery without auxiliaries and solvent based on the key components cellulose, xylose and lignin of 1 ton fresh matter feedstock. The product flows represent pure components

TABLE 1 Assumptions for the TEA

Scale-up capacity range: (miscanthus input with 10 wt.% dry matter)	Total plant cost:
<ul style="list-style-type: none"> • Scale 1: 0.5 tons per hour • Scale 10: 5 tons per hour 	<ul style="list-style-type: none"> • Equipment cost • Other direct costs (specified as % of equipment cost) <ul style="list-style-type: none"> ◦ Installation: 39% ◦ Piping: 31% ◦ Instrumentation: 26% ◦ Building and structure: 12% ◦ Auxiliaries: 55% ◦ Outside lines: 5% ◦ Indirect costs (specified as % of equipment cost + direct costs) <ul style="list-style-type: none"> ◦ Engineering and Construction: 65% ◦ Legal expenses: 4% ◦ Contractor's fee: 19% ◦ Contingency: 37%
The techno-economic profitability factors:	Manufacturing costs:
<ul style="list-style-type: none"> • Biorefinery lifetime: 20 years • Operation time: 7.000 h per year • Equity: 30% • Debt interest rate: 3% • Equity interest rate: 10% • Depreciation period: 10 years • Depreciation method: Straight line depreciation • Fixed costs, raw material and product prices increase by 1% per year 	<ul style="list-style-type: none"> • Labor expenses: <ul style="list-style-type: none"> ◦ Direct cost: 4 shifts ◦ Indirect cost: 20% of direct cost • Tax and insurance: 2% of Total plant cost • Maintenance: 4.5% of Total plant cost
Working capital: 10% of total revenue	
Tax: 30% on income	
Reference year: 2020	
Price index: PCDI	

Concerning the mass flow for miscanthus \times giganteus, the composition analyses show a lignin content of 12 wt.% dry matter, cellulose contents of 49 wt.% dry matter and hemicellulose contents of 28 wt.% dry matter. The amount of biomass needed is derived from the EU-BBI-GRACE-project. The material balance consists of ash, proteins and an analytically undeterminable remainder. The water content is approximately 9.7 wt.%. Thus, one ton of fresh miscanthus contains 805 kg of the key components lignin, hemicellulose and cellulose (see Figure 3).

In the pretreatment module M 1, the cellulose is partially hydrolyzed. The crystalline cellulose is not solubilized under these conditions (Paksung et al., 2020) and is discharged together with the lignin. The hemicellulose is converted only to the amount of xylose to simplify the process simulation. This results in a gap in the mass balance, which is shown as an accumulated rest flow depicted as a gray line in the Sankey Figure 3. This includes other hemicellulose components such as arabian or galactan. The gap in the mass balance after M 1, which is not covered by the defined key components and is caused by different analytical methods and the normalizations in the simulation, is 5.5 wt.% or 44.4 kg.

In addition to the solids, some of the glucose and xylose and some of the rest flow are also transferred to module M 4. The solids are still moist and therefore a proportion of the dissolved substances is also discharged. In this process step, the coal yield is very high compared to the phenol yield. There is a need for further optimization here. The glucose, xylose and residual material streams that have been dissolved in M 1 are subsequently converted to furfural and HMF in M 2A and M 3A, respectively, and

purified and separated in M 2B and M 3B. As already described in the assumptions for the Aspen simulation, a solid formation of 10 wt.% related to the starting carbohydrates is assumed. In the continuous test setup of the pilot plant, an exact determination of the coal formation is not possible. Analogous to M 1, further compounds are also formed during the subsequent reactions, which are again summarized here as a rest. The missing components to fill the gap to 100% in the mass balance are side products, that have not been individually included in the simulation. The publication by Wüst et al. (2020) summarizes these possible reaction side products. The reactors in M 2 and M 3 are not operated at full conversion so that unreacted xylose and glucose remain in the process water. In the process simulation, 90 wt.% of these are returned to the reactor (M 4B to M 1). This increases the overall yield, producing 95 kg of HMF and 117 kg of furfural from 1 ton of miscanthus. The missing 10 wt.% is removed from the cycle by a purge stream toward the biogas plant to avoid accumulation of dead-end compounds, salts and other impurities.

With one distillation unit, only a certain proportion of the furfural produced can be separated from the process water in M 2B at the desired purity. However, since furfural is hardly decomposed in aqueous, acidic media and under the influence of temperature (Dunlop, 1948), this is also recovered so that the furfural losses are only a result of the purging process. Here, an additional process sub-step, such as stripping unit or a second distillation unit could further reduce the furfural losses if necessary. In the case of HMF, a tolerable loss of 2 wt.% of the HMF quantity is assumed, since HMF subsequently reacts easily further to, for example, hydrochar and levulinic acid (Jung

		Materials	Value
Input	M 1	Miscanthus	500 kg/h
		Water	656 kg/h
		Acid	0.3 kg/h
		Heat	3332 MJ/h
		Power	23 MJ/h
	M 2	Heat	4107 MJ/h
		Power	2 MJ/h
	M 3	Auxiliary 1*	2.2 kg/h
		Auxiliary 2*	43.4 kg/h
		Heat	1235 MJ/h
		Power	20 MJ/h
	M 4	KOH	3 kg/h
		Ethyl acetate	13.9 kg/h
		Heat	1155 MJ/h
		Power	34 MJ/h

		Products	Value
Output	Heat	1.646 MJ/h	
	Furfural	61.5 kg/h	
	HMF	52 kg/h	
	monomeric aromats	10 kg/h	
	Char wet	339.5 kg/h	
	Rest to biogas plant	671 kg/h	
	Auxiliary 1*	2.2 kg/h	
	Auxiliary 2*	43.4 kg/h	
	Ethyl acetate	13.9 kg/h	

FIGURE 4 Input and output values of the small-scale biorefinery (500 kg/h). HMF purity, 0.9 wt.%; Furfural purity, 0.95 wt.%; Phenolic compounds purity, 0.9 wt.% and a moisture content of the char of 57 wt.%. *Details cannot be described because of a current patent application

et al., 2021). This leaves the plant via the purge stream toward the biogas plant.

In summary, with this plant configuration and the assumptions made at the current stage of development, 95 kg of HMF, 117 kg of furfural, 18 kg of a phenolic monomers, 75 kg of HTC char and 217 kg of a solid mixture of lignin, char and carbonized crystalline cellulose can be recovered from one ton of miscanthus. Due to rounding and the internal uncertainties of the various analysis methods, the mass balance cannot be completely closed. The missing 42 kg correspond to 5.2% related to the described input key components. Regarding the uncertainty of miscanthus composition by comparing analytical and literature data (Arundale et al., 2015), the cellulose, hemicellulose and lignin contents vary by more than 20 wt.%. The composition is mainly affected by, for example, the cultivation location or the genotype and results in corresponding variations in product yields. This composition variation is taken into account in the upcoming sensitivity analysis (see Section 3.5).

The input and output material and energy flows are summarized in Figure 4 of the small-scale biorefinery with a capacity of wet biomass of 500 kg/h in steady-state, running operation. The plant is completely filled and Figure 4 shows the mass flows leaving and replacing the biorefinery per operating hours sorted by modules. Differences between input and output flows occur because of rounded

numbers. Compared to Figure 3, Figure 4 includes the solvent water, the auxiliaries and the power and heat demand.

3.2 | Cost estimation

The baseline states the cost estimation results of the Scale 1 biorefinery. Based on the unit operations used in the process simulation, the main components of the plant were defined and the capital cost estimated. The estimate of the investment level for these apparatuses is presented in Table 2 and shows the aggregated equipment costs after price and currency adjustment to the year 2020, including scaling factors and labor requirements. The highest equipment cost of approx. 0.89 Mio. EUR has the furfural production module (M 2) followed by the HMF production module (M 3) with 0.42 Mio. EUR and the phenol production module (M 4) with 0.28 Mio. EUR as well as the pretreatment module with 0.27 Mio. EUR. The equipment cost of the modules amount to 1.8 Mio. EUR. The most labor-intensive module with 0.64 of personnel required per shift is the HMF production (M 3). In the supporting information, the distribution is shown again as a pie chart.

Further cost for the storage and internal transport of the raw materials as well as utilities or operating materials for the cooling circuit and the heating of the plant are

TABLE 2 Estimation of the acquisition costs of individual plant apparatus of the Scale 1 biorefinery

Module	Equipment	Number	Cost [T EUR]	Scale-up exponent	Labor factor ^a
M 1	Pumps ^b	2	278	0.6	0.4
	Biomass pre-treatment ^a	3		0.6	
	Heat exchanger ^a	2		0.6	
	Reactor ^c	1		0.9	
	Separator ^b	1		0.9	
M 2	Heat exchanger ^a	4	886	0.6	0.38
	Reactor ^b	1		0.9	
	Filters ^a	2		0.6	
	Distillation column ^b	1		0.55	
	Decanter ^d	1		0.6	
M 3	Pumps ^a	2	413	0.6	0.64
	Heat exchanger ^a	4		0.6	
	Reactor ^b	1		0.9	
	Filters ^a	2		0.6	
	Separation units	1		0.68	
M 4	Pumps ^a	3	282	0.6	0.48
	Heat exchanger ^a	4		0.6	
	Reactor ^b	1		0.9	
	Filter ^a	2		0.6	
	Mixer-Settler ^a	1		0.6	
	Distillation column ^b	1		0.55	
	Tank ^a	1		0.6	
Total			1.8 Mio. EUR	2 per shift	

^aBrown (2006).

^bPeters et al. (2003).

^cChauvel et al. (2003).

^dTrippe (2013).

independent of the modular process simulation and are summed up to 0.2 Mio. EUR. Hence, the sum of equipment cost results in a total of approximately 2.0 Mio. EUR for the Scale 1 biorefinery.

In addition to capital cost for the major components of the plant, further capital expenditures were calculated based on the TEA assumptions (Table 1) using the factor method. Within inside battery limits, the capital cost estimation figures for a brownfield biorefinery approach result in a total of approximately 5 Mio. EUR.

The annual operating costs (OPEX) of the plant are divided into variable and fixed costs. The variable operating costs include the supply and transport of miscanthus and the synthesis and purification steps to produce the final products as well as the disposal of the waste streams into a biogas plant. The flows of electrical and thermal energy were determined in accordance with the process simulation (c.f. Figure 2).

The overall operating cost per year amount to 2.3 Mio. EUR of which the variable operating costs account for 59%

and the fixed costs for 41%, which contain fixed labor and overhead as well as maintenance and tax and insurance.

By assuming a miscanthus price of 90 EUR per ton (Petig et al., 2019), the provision of feedstock has a share of 14%, as seen in Figure 5. The labor and overhead costs account for 32% of total operational expenditures and consist of direct personnel costs of 27% and indirect personnel costs of 5%. The labor hours amount to 18,790 labor-hours per year for the Scale 1 concept and were estimated using labor equivalents for selected major components after a literature comparison (Brown, 2006; Peters et al., 2003, 2004). The high labor requirement of two persons per shift are justified by the assumption that optimized automation of the plant concept has not yet taken place and should be investigated in follow-up studies.

The highest cost share with 12% of the four modules accounts to module M 3. The other modules share is between 8% and 9%. In total, the modules are attributable to 37% to the OPEX. Of this, the largest share is for heating costs, followed by auxiliaries and miscanthus costs. The

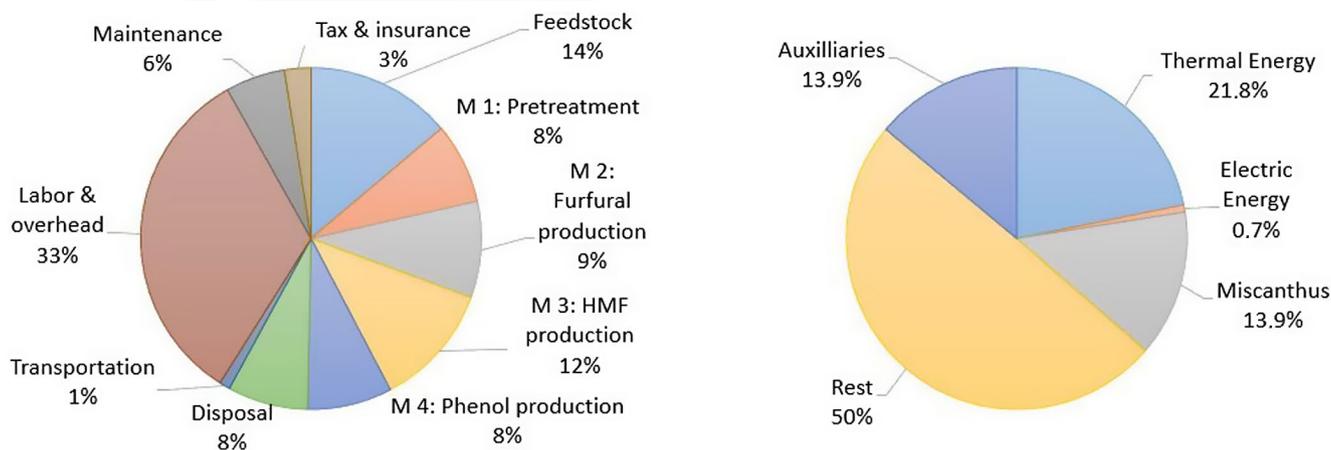


FIGURE 5 Distribution of total OPEX costs of the biorefinery in Scale 1 (500 kg/h) per module (left) and per input (right)

scale-dependent transport costs are determined depending on the annual transported quantity to satisfy the demand at the plant according to its capacity and amount to roughly 1% after Eltrop et al. (2014).

Due to the spatial distribution, biomass has higher supply and transport costs with increasing transport distance, which leads to negative economies of scale and can be referred to as diseconomies of scale or more specifically diseconomies of supply. This effect is more pronounced the larger the planned plant concept is and counteracts the classic economies of scale. In the present case, this effect plays a subordinate role due to the small plant sizes and the short transport distances, but requires demonstrative investigations for larger distances.

3.3 | Scale-up

Based on the baseline cost estimation of the basic plant design, a scaling-up of the plant concept is performed. To allow for gradual scaling starting from Scale 1 to Scale 10, individual apparatuses were assigned with specific scale-up factors.

With scale increase, the total capital costs rise disproportionately with a scaling factor of approx. 0.63. This disproportionate increase characterizes the classic economies of scale in process engineering, which often has a value between 0.5 and 0.7 for thermochemical processes (Turton et al., 2008). The scaling factor of 0.63 consists of individual scaling factors of each of the modules. The scaling factor of the pretreatment module (M 1) is 0.74. The furfural production module (M 2) has a scaling factor of 0.59, the HMF production (M 3) of 0.69 and the phenol production of 0.63 (M 4).

Compared to the total capital costs of the Scale 1 concept with 5 Mio. EUR, a 10-fold increase in capacity results in a roughly fourfold increase to 21 Mio. EUR in the Scale 10 concept. The operating costs, however, have

almost seven-folded from 2.3 to 15.8 Mio. EUR. Thus, the OPEX-scaling factor is 0.85. Figure 6 shows the degressive development of the absolute CAPEX and the share of OPEX for the 10 scales.

As expected, the share of transportation costs increases with higher biomass demand. The scale increase significantly reduces the OPEX, in particular the portion of direct personnel cost, from 27% (scale 1) to 7% (scale 10). For those small scales, the personnel requirement of 2.47 per shift (scale 9) is unsuitable and must be assessed as too high. Other on-farm biorefinery concepts such as biogas plants calculate with far lower personnel demands. A rule of thumb here is 6.7 working hours per kilowatt and year (Schattauer & Weiland, 2006). With an average plant size of 415 kW in Germany (Daniel-Gromke et al., 2017), this is just 2780 h/a, instead of 23 thousand working hours assumed in this work.

Positive economies of scale in the economic evaluation of process engineering systems describe the effect of disproportionate increase in equipment costs of system components with component size. Thus, the specific capital costs do not decrease linearly with an increase in the plant capacity, but degressively from a capacity exponent lower than one. The closer the scaling factor is to the value one, the lower the scaling effects. Exponents of degression (scaling factor) in size close to one thus favor decentralized biorefinery concepts, since a reduction in the specific production costs per output unit is small and would be zero with an exponent of one. Put simply, a high exponent value (close to one) speaks for a numbering-up, that is, the decentralized installation of several small systems, and a value well below one for a scale-up of the systems, that is, the centralization of production capacities to a few large systems.

In the economic evaluation of process engineering plants, the decisive factor is which type of conversion processes are used. A factor of 0.63 as for the baseline cost estimation enables to operate small biorefineries economically. However, this value is not high enough to argue as a

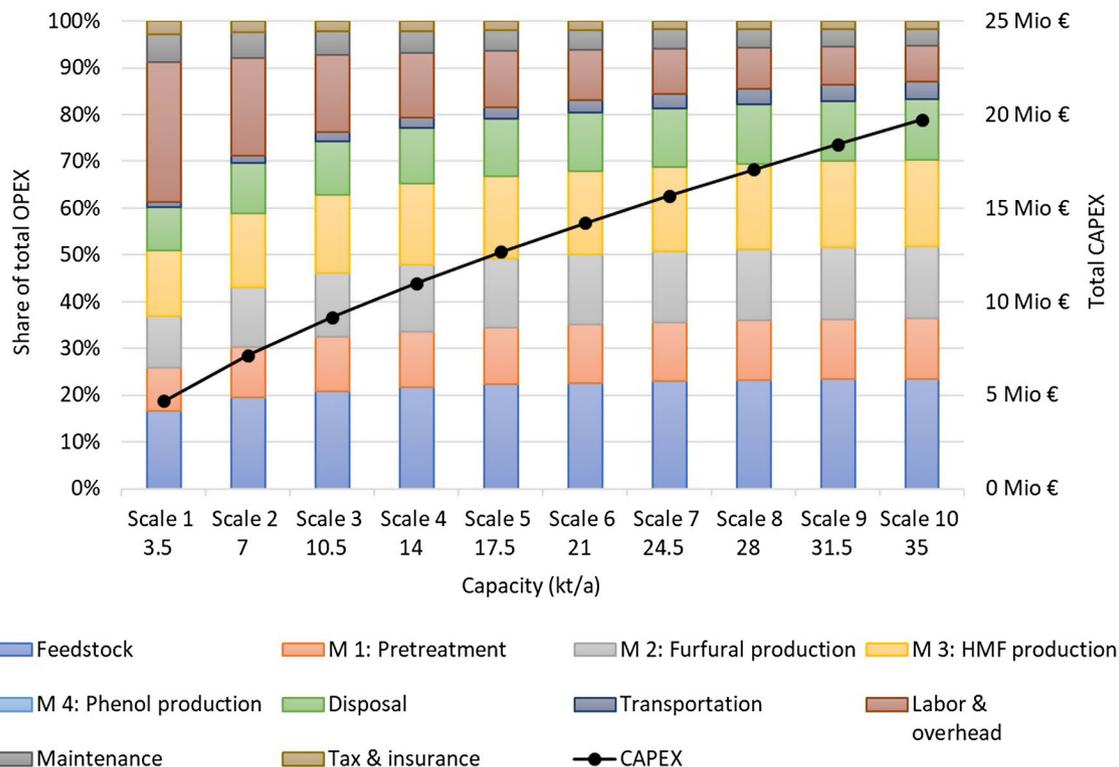


FIGURE 6 Development of the share of annual operating costs within the biorefinery capacity limits depending on the scale

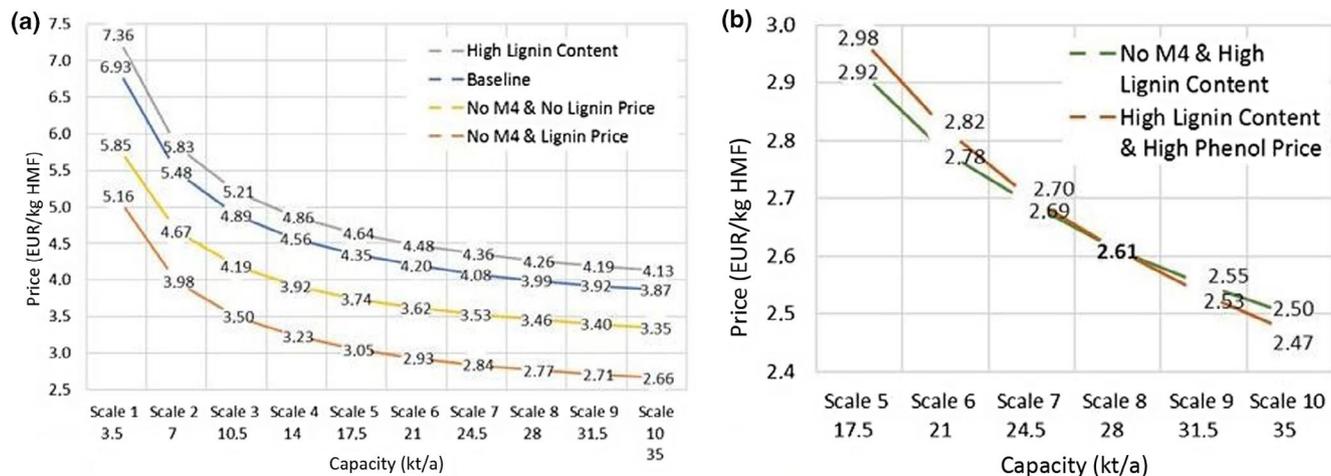


FIGURE 7 (a) HMF price plot of different scenarios over a scaled plant size from 3.5 to 35 tons of miscanthus input per year. HMF price plot comparing two scenarios with high lignin content over a scaled plant size from 17.5 to 35 kilo tons of miscanthus input per year. (b) No M4 = no valorization of lignin to monomers; High lignin content = miscanthus feedstock has a lignin content of 21 wt.%; High phenol price = minimum selling price of 6 EUR/kg monomeric aromats instead of 1.3 EUR/kg

standalone argument for numbering-up and thus smaller, decentralized plants, or the other way around.

3.4 | Scenario analyses

The scale-up results are used in the following scenario analyses and provide a price range of 3.87–6.93 EUR/kg HMF (c.f. Figure 7a), while the prices of all other products

are kept constant (cf. Supplementary Materials S1). These calculation figures are applied in an analysis with three scenarios to derive to the optimal plant capacity and biorefinery configuration. The first scenario “High Lignin Content” assumes a higher lignin content of miscanthus. Whereas the second scenario “No M4 & No Lignin Price” describes a concept configuration without the phenol module M 4, the third scenario “No M4 & Lignin Price” as well removes M 4, but sells lignin additionally.

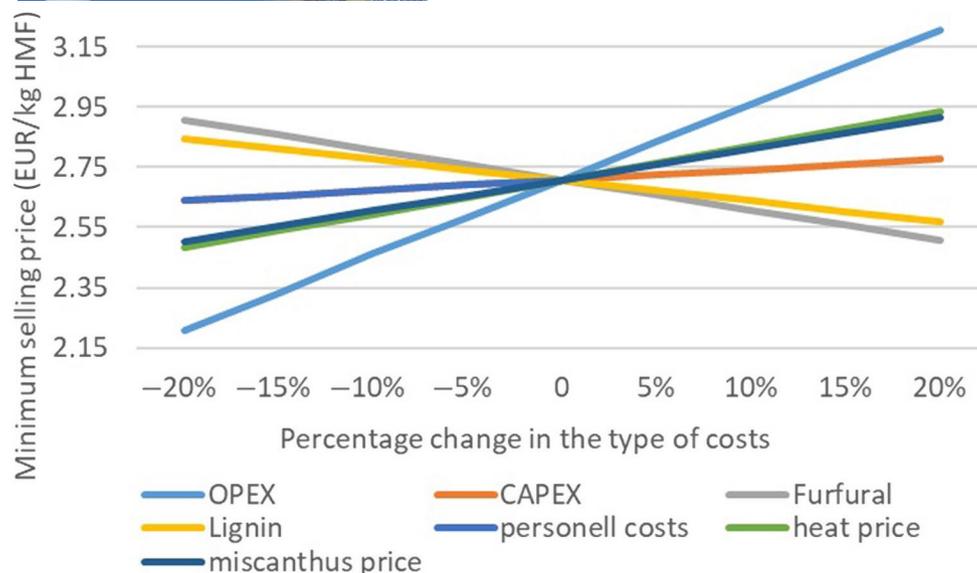


FIGURE 8 Sensitivity analyses of CAPEX and OPEX, furfural and lignin prices as well as personnel costs, heat price and the miscanthus price on the HMF minimum selling price

The High Lignin Content scenario relates to the aforementioned uncertainty in miscanthus composition (cf. Section 3.1) and considers a higher lignin content in the miscanthus composition of 21.4 wt.% wet based according to Butler et al. (2013). Especially, lignocellulosic biorefineries require the utilization of lignin to be economically feasible (Petig et al., 2018). The goal of this high lignin content scenario is to investigate whether lignin utilization is a key factor for the economic viability of the proposed miscanthus biorefinery. Increasing the lignin content in the biomass decreases the hemicellulose and cellulose content. This changes not only the product quantity of the phenolic mixture, but also the HMF and furfural quantity. The corresponding data are provided in Supplementary Materials S1. By keeping the CAPEX and OPEX equivalent to the baseline figures, the minimum selling price of HMF for Scale 10 is 4.13 EUR/kg HMF as shown in Figure 7a by the gray-dotted line.

The No M4 & No Lignin Price scenario removes module M 4 and assumes that the lignin slurry is not valorized. This leads to a reduction of CAPEX from 20 to 18.5 Mio. EUR and a CAPEX scaling factor reduction to 0.62 in comparison to the baseline. Without module M 4, lower HMF prices can be achieved ranging from 5.85 to 3.35 EUR/kg HMF as shown in Figure 7a by the yellow-dotted line.

The No M4 & Lignin Price scenario removes module M 4 of the biorefinery and sells lignin at a price of 0.6 EUR/kg (Smolarski, 2012). This lowers the HMF price further as shown in Figure 7a by the red-dotted line. The input-output tables for the No M4 scenarios are also attached in Supplementary Materials S1.

Concluding findings highlight that the timing of miscanthus harvest should minimize the degree of lignification at maximum dry matter yield.

By comparing the two lignin valorization scenarios with another where both scenarios assume a higher lignin content and either a high lignin price of 0.6 EUR/kg (No M4 & High Lignin Content & Lignin Price) or a high phenol price of 6 EUR/kg (High Lignin Content & High Phenol Price), an assessment of the cost-effectiveness of the M 4 module is possible (shown in Figure 7b).

For example, by either selling phenol mixture at a very high price or by further lowering the cost of the phenol module M 4. In general, the sales can be increased with higher product yields by moving the semi-continuous setup to a continuous plant design and recycling of the unreacted lignin fragments. While the OPEX can be reduced by lowering the consumption of ethyl acetate, for example, by applying a countercurrent extraction for the separation (M 4B), as explained in detail in chapter 8 the CAPEX do not have a major effect on the product prices (see Figure 8). Hence, future research shall focus on reducing solvent consumption and on the recovery of unreacted lignin. At the current stage of development (TRL 3–4), this has not yet been the focus of research. Increasing the TRL to 6, the same TRL of the other modules, would strengthen the validity and comparability between the scenarios.

If the plant size of the presented biorefinery concept is restricted, for example, by low biomass availability at the site, a plant capacity to the left of the crossing point at Scale 8 of the two lines is favored without the implementation of module M 4 as in the No M4 scenario. Instead, the valorization of lignin could be done by semi-decentralized concepts similar to dairies. For larger plant sizes, decentralized on-site refining of lignin to phenol mixtures becomes more economical.

Using the HMF price as an indicator, the scenario results lead to a concept configuration with a process combination containing the modules M 1, M 2, M 3 and M 5 without further refining of lignin to phenolic compounds. Given a continuous supply of miscanthus and by comparing the payback period, an optimal concept size with a capacity of roughly 31.500 tons per year can be determined. As investigated by Petig et al. (2019), several regions in Baden-Württemberg can provide the required miscanthus quantities for the addressed capacity ranges within a supply distance of only a few kilometers.

If the above-mentioned variable heat and miscanthus prices and quantities are not a limiting factor, the decision on the plant size depends on aspects such as product market volume, committed purchase quantities and available capital that required further investigation. Due to the regressive curves (see Figure 7a), slightly lower minimum selling prices are still achievable with a Scale of 10 compared to Scale 9. But the payback period decreases from 16 to 13 years between Scale 1 up to Scale 9, but does not decrease further from plant size 9 to 10. Smaller plants require less capital and the break-even volume is lower. The risk of losses is thus reduced. This is a critical argument for small-scale biorefineries, especially when piloting new processes and technologies.

3.5 | Sensitivity analyses

For the optimal plant configuration without M 4 and by assuming a high lignin price such as in scenario No M4 and Lignin price, a sensitivity analysis is used to identify the most critical parameters that most effectively lead to a price reduction of HMF. For this purpose, the CAPEX and OPEX as well as the prices of the co-products furfural and lignin are varied in five steps from/to $\pm 20\%$. The results of the parameter variation are shown in Figure 8.

If one looks at the range of variation with changed market prices of the co-products, this amounts to a maximum of 7.3% for furfural (*ceteris paribus*). Within this range, CAPEX have an influence of $\pm 2.5\%$ at most, whereas OPEX can influence the HMF price by $\pm 18.5\%$. This leads to the conclusion that the greatest optimization potential lies in a reduction of OPEX and, for example, not so much in a technical optimization of the main apparatus. To be able to assess the economic efficiency at the current stage of development, OPEX that are not directly related to the technical process are selected for the further sensitivity analyses (Figure 8). The cost items personnel requirement, heat price and miscanthus price are more technology-independent than, for example, the items auxiliary material and heat quantity. While personnel costs are overestimated, only a cost reduction is considered.

To reach a higher reduction in personnel costs than 20%, the degree of automation of the industrial plants should be much higher than currently in the biorefinery baseline scale. Here, one can take the example of on-farm biogas plants. These can be operated by the farmers' employees themselves. In principle, there would then only be a need for skilled staff for maintenance and repair work. This could be organized through service contracts for several decentralized biorefineries, which would lead to a massive reduction of the OPEX. The authors are of the opinion that a joint reduction of heat and miscanthus costs to this extent (-20%) is at least achievable and they see a combination of these scenarios as already realistically feasible independently of further technical optimizations on the way to industrial maturity (TRL 9). Overall, including personnel costs reduction by 20%, this would reduce the HMF price to 2.21 EUR/kg.

Concerning the heat prices, a study published in 2018 reports extremely heterogeneous prices for heat delivery from biogas plants. These vary from free provision to over 10 EUR cents/kWh (Herbes et al., 2018). Even with a small-scale biorefinery and thus an on-site biogas plant, the costs for heat supply have to be considered. Favorable and long-term purchase contracts can significantly reduce HMF prices. It is also recommended to not operate the biorefinery mostly during winter times when the heat is needed elsewhere, for example, in stables. The part of technical optimization of energy and material coupling of small-scale biorefineries with biogas plants is currently the subject of further research.

Regarding the feedstock prices, a study on the price-driven feedstock potential of miscanthus in Baden-Württemberg identifies regions, even at prices of 72 EUR/ton, that could provide enough feedstock for the biorefinery to produce HMF at a price per kilogram of 2.21 EUR/kg (Petig et al., 2019). These values can only be achieved by assuming a lignin price of 600 EUR/ton. Whether the lignin quality is sufficient for this price requires further research. To address this uncertainty, a sensitivity analysis of -20% for the raw material costs, heat and personnel costs are again applied to Scale 9 of the worst-case scenario in which the lignin is not a marketable product and has no sales (No M4-No Lignin price scenario, Figure 7). The resulting minimum selling price for this scenario would be 2.90 EUR/kg HMF. As a result of this work, we see a price range of 2.21–2.90 EUR/kg HMF as realistically achievable.

A study of FNR showed that the material prices of biobased and biodegradable plastic goods are 2–3 times higher than that of competing petrochemical materials (Rohstoffe eV FN, 2014). This is aligned with our findings of a HMF market price of approximately 2–3 EUR/kg compared to the fossil equivalent for polyester production of 0.85 EUR/kg para-xylene (Davidson et al., 2021). To enter the market rapidly HMF must be converted into

customer goods with advanced functionalities such as polyethylenefuranoate PEF, which has better barrier properties compared to PET (Burgess et al., 2014). However, the presently high prices of HMF combined with the low market availability may hinder rapid product development. Nonetheless, biobased product potentials for higher value applications will increase and, in the mid to long term, regulatory requirements such as the CO₂ taxes are expected to cause the price of fossil raw materials to rise. This will further close the gap between the prices of fossil-based and biobased chemicals.

In its configuration of a sucrose HMF plant, Steinbach assumes production costs of 4.30 EUR/kg (Steinbach, 2020). Regardless of the underlying technology maturity, starting biomass, reaction media and calculation methods used, Davidson et al. (2021) show HMF prices ranging from 0.35 (minimum production costs, not price) to 2.16 (minimum selling price) \$/kg in a review article published in 2020. With prices between 2.21 and 2.90 EUR/kg, we are just out of the range. But even though, the authors see the process as competitive because it is already being tested and further developed on a pilot plant scale. Also, the implementation in an aqueous medium (green chemistry approach) makes decentralized, regional operation possible without major infrastructure requirements. In addition, the use of carbon-positive second-generation biomass such as miscanthus incorporates a socially acceptable sustainable concept.

4 | CONCLUSION

Biorefinery concept is the key for the bioeconomy, but its viability requires economic evaluation while taking different scales and configurations into account. Financial feasibility in terms of profitability is the major problem of bioproducts production. To improve the competitiveness, the end-product prices must be further lowered through further process engineering developments toward industrial production.

For example, for the modules M 1–3, the idea of lower reaction temperatures at the same yield through longer residence times could also be considered. This may reduce the overall energy demand to some extent and thus mitigate some of the uncertainty with respect to the heat price. The prerequisite for this, of course, would be a similar yield and quality of products. Especially concerning real input biomass, there is some further research needed. Also, the assumption to purge 10 wt.% of the total flow of the recycling loop has to be validated and if possible minimized. By reducing the purge-stream, more carbohydrates can be recovered. This task must be tackled in a first of its kind demo plant at industrial scale.

Next to process optimization, the profitability of biorefinery concepts is influenced by market potentials of biobased product, which in contrast to fossil-based products provides functional benefits through better material properties and better sustainability. For instance, a market study showed that the biobased, biodegradable and more expensive mulch film in agriculture led to an unexpected manifestation in the market because of its property to be decomposable (Rohstoffe eV FN, 2014).

The analysis of the OPEX distribution, the scaling and the sensitivity analyses have shown that the question of the optimal plant size and configuration depends mainly on the geographical features of the facility as well as the local heat and feedstock prices. Nonetheless, further decision criteria like population, social or industrial factors must be taken into account by considering multiple criteria simultaneously.

It was also found that the personnel costs have a major impact on the minimal selling price of HMF. But the results indicate that the common methods for calculating personnel requirements rely on historical data of fossil industries. For small-scale biorefineries, they are not fully suitable. They tend to overestimate for smaller scales. The authors see a need for further research and optimization for the evaluation of personnel costs for agro-industrial “on-farm biorefineries.”

Therefore, future research must pose the biorefinery concept evaluation into a multi-objective optimization problem. The environmental impact of the biorefinery concept will be discussed in an upcoming publication.

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DATA AVAILABILITY STATEMENT

Raw data material is available after request at Zenodo.org under <https://doi.org/10.5281/zenodo.5838719>.

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SUPPORTING INFORMATION

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