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Simultaneously optimizing the capacity and configuration of biorefineries

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Advanced biomass conversion plants can replace fossil resources in the electricity, heat, transportation fuels and chemicals sectors, but they face specific challenges with regard to their economic operation. When choosing a capacity for a biomass conversion plant, economies of scale must be weighed against the transportation costs for the widely-distributed input materials.

Here, we model the problem of determining the optimal capacity for plants with a single product or a fixed set of products using a single optimization variable and two alternative economic objective functions. To identify the factors that most strongly influence economic plant operation, we perform a sensitivity analysis of various model parameters to determine their impact on the optimal solution using the Envelope Theorem. We also present an optimization approach for simultaneously planning the capacity and configuration of multi-product plants. By modeling economies of scale on a process-specific level, our nonlinear optimization approach makes it possible to determine the optimal configurations, and thus ranges of products, for changing plant capacities. An examination of the obtained feasible solutions shows that the optimization problem is neither convex nor concave.

1.1 Introduction

Biomass is generally considered the most versatile renewable resource due to its suitability for electricity generation, heat supply, transportation fuels, and chemicals production. Instead of using crops such as corn, canola or sugar beet merely to produce individual products like bioenergy or fuel, multi-product approaches are often promoted to use the existing biomass as efficiently as possible (Kamm and Kamm, 2004). Among the main advantages of plants that use biomass as both energetic and material feed stocks, such as biorefineries, are the efficient use of as many biomass components as possible and the generation of renewable carbon input materials for the process industry (Bozell, 2008). Residuals from forestry and agriculture are frequently considered as feed stocks for such plants, since they have fewer competing uses.

The location and capacity planning of biomass conversion processes is complicated by the fact that biomass is distributed quite evenly throughout fertile areas of the earth's surface

(Ekşioğlu, Acharya, Leightley, and Arora, 2009). Thus, unlike coal, mineral oil or natural gas, it cannot be extracted locally. Although a similar situation also prevails in some other sectors of forestry and agriculture, the low value of residual biomass means that efficient supply structures are especially important for the processes designed to use them. Unless biomass can be imported by ship or extracted from large-scale municipal waste facilities, the specific cost of transporting biomass often limits biorefinery capacities (Ekşioğlu et al., 2015; Heffels, et al., 2014; Overend, 1982). Since a larger catchment area is required for big plants than for small ones, the transportation distances and specific transportation costs rise with plant capacity. To deal with this complication, one needs suitable models to determine optimal capacities.

Due to the large number of concepts for converting finite quantities of specific kinds of biomass into valuable products, one must also make choices about the best conversion pathway. These choices include the selection of technologies and capacities, the target products and the most suitable biomass inputs for the entire planning horizon.

Among biomass conversion plants, biorefineries are considered promising opportunities to enhance the business opportunities of existing companies in the biomass sector (Mansoornejad et al., 2010), a fact that is also emphasized e.g. in the American, German and Finnish bioeconomy strategies (Germany: Federal Government, 2014; Ministry of Employment and the Economy, Finland, 2014; US government, 2012). A recent overview of national definitions and applications by the International Energy Agency (IEA) resulted in the following, relatively broad definition: “Biorefining is the sustainable synergetic processing of biomass into a spectrum of marketable food and feed ingredients, products (chemicals, materials) and energy (fuels, power, heat)” (IEA, 2014). However, a more specific German definition -- also cited in the IEA overview -- is formulated thusly: “The biorefinery process chain consists essentially of the pre-treatment and preparation of biomass, as well as the separation of biomass components (primary refining) and the subsequent conversion and processing steps (secondary refining)“ (Germany: Federal Government, 2012; IEA, 2014). This distinction, which may have been made due to issues relating to the granting of subsidies by excluding most existing bioenergy plants from being eligible for subsidies targeting biorefineries, divides biorefineries into two distinct parts. Since the primary refining section of a biorefinery always yields the same intermediate, the production of marketable products resides entirely in the secondary refining section.

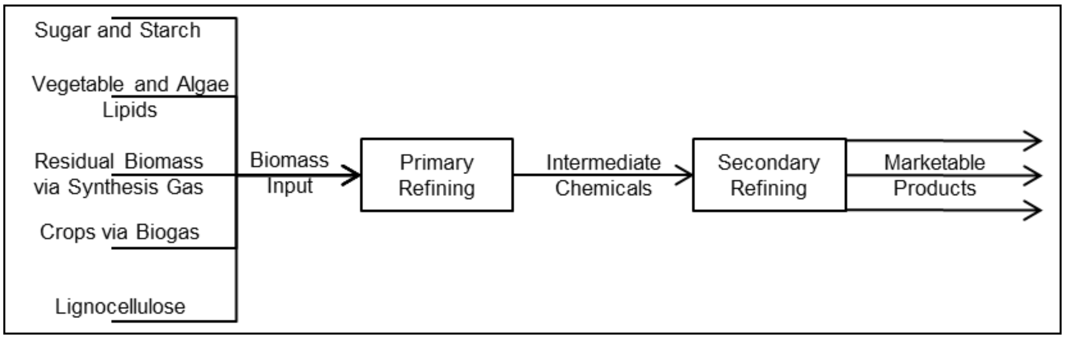

Figure 1: Schematic representation of a biorefinery defined according to (Germany: Federal Government, 2012)

Figure 1 schematically illustrates the sequence of primary and secondary refining processes in a biorefinery based on any of the biorefinery concepts discussed in (Germany: Federal Government, 2012). Primary feed stocks include sugar and starch, vegetable and algae lipids, synthesis gas, biogas and lignocellulose. Following this definition, the range of products exiting the planned biorefinery is a result of the upgrading and separation processes in the secondary refining section--also referred to as the section's configuration. A decision must be made about which substances are to be blended into fuel (Trippe et al., 2013) (i.e., after upgrading) and which are to be sold as purified chemicals (i.e., after separation). This decision is complicated by the fact that the relative advantages of the various options depend on the capacity of the conversion facility as a whole, since some processes benefit more from economies of scale than others.

Capacity optimization for both mineral oil refineries and biomass conversion plants has been discussed repeatedly in the past. The development of transportation distances to deliver biomass to plants of different capacities was analytically investigated by Overend (1982). A nonlinear optimization approach was applied by Jenkins (1997), who assumed a rectangular catchment area around the plant to approximate transportation distances and costs. The objective function was designed to minimize the unit prices of a biomass conversion plant. In contrast, Cameron et al. (2007), Caputo et al. (2004) and Wright and Brown (2007) assumed a circular catchment area, such that the specific transportation cost of the input biomass per ton of production capacity is proportional to the square root of the plant size (Kumar et al., 2003). If the total transportation cost for input biomass is expressed as a function of plant size, an exponent of 1.5 is usually assumed for the resulting term (Lauven, 2014; Wright and Brown, 2007). The resulting nonlinear correlation between plant capacity and biomass transportation cost can modeled with nonlinear equations for biomass conversion plants in order to analyze interactions between different influencing factors. Due to the growing interest in such plants, it is worth investigating whether methods from Operations Research, such as nonlinear programming algorithms, might also help to reliably solve this particular problem.

Rentizelas et al. (2009) attempted to tackle the nonlinearities in such models by using a hybrid approach. This consisted of Genetic Algorithms (GA) and sequential quadratic programming (SQP), which "may lead to the identification of the global optimum" of nonlinear (or, more specifically, nonconvex) problems. Other approaches have focused on location or network planning. These use mixed-integer linear programming techniques for ethanol plants (Leduc et al., 2010) or more complex biomass conversion processes, such as Biomass-to-Liquid plants, with decentralized pre-treatment units (Walther et al., 2012). More recently, planning approaches have focused on the design of biorefineries. Toward this end, the process engineering software ASPEN Plus has been combined with metaheuristics and linear programming models to investigate optimal biorefinery configurations and operating conditions (Geraili et al., 2014a, 2014b). These models optimize the actual operation of individual chemical conversion processes in biorefineries instead of merely choosing from potential alternative process options.

One must weigh alternative process options if the choice of conversion processes, and therefore of the product portfolio, is still unclear. The approach proposed here focuses on a point in time at which it is still unclear which plant sizes and upgrading processes will be the most beneficial for a biorefinery. We focus on answering the following research question: Can an integrated capacity and technology choice modeling approach based on nonlinear programming help to plan biomass conversion plants with several potential products and widely distributed biogenous inputs?

This modeling approach includes economies of scale calculations for individual secondary refining processes and thus allows plant capacity and configuration to be optimized simultaneously. We illustrate our approach by planning (in Germany) a biorefinery that assumes synthesis gas from residual biomass to be the intermediary substance. Without major adaptations, however, the same approach could be applied to the corresponding primary and secondary refining sections of biorefineries based on other inputs (see Figure 1) and on different plant locations. Since the number of potential biorefinery products is quite large--even for a given biomass input--the optimization focuses on the configuration of the secondary refining section. Here, the best configurations may result in a total product value several times higher than that of less well-configured plants. In contrast, primary refining is far less variable and thus offers less optimization potential from a configuration modeling point of view—this, despite the fact that primary refining causes the greater part of the investment and contains more technical challenges (Boerrigter, 2006).

This paper is structured as follows: In Section 1.2, the nonlinear optimization approach for plants with a fixed configuration is described to introduce the choice of both profit and return on investment maximization as objective functions. Then, the modeling approach is extended to permit variable configurations as part of an integrated capacity and configuration planning for biorefineries. In Section 1.3, the resulting nonlinear optimization problem is applied using parameter values for Germany. After solving for the fixed configuration, a sensitivity analysis is conducted to show the influence of parameter value changes on the optimal plant capacity. The variable configuration model is also applied and the structure of the optimization problem is investigated. Section 1.4 contains a critical analysis of the various solutions. Finally, in Section 1.5, we conclude the paper with a look at possible extensions of our approach.

1.2 Nonlinear optimization of biomass conversion plants

The economic competitiveness of a biomass conversion plant can be measured by approximating such performance indicators as the prospective profits, the return on investment (ROI), the internal rate of return (IRR) or the net present value (NPV). Because the main advantage of the dynamic methods involving IRR or NPV is the more detailed inclusion of estimates for future income and expenses, their additional utility depends greatly on the accuracy of these estimates. In the energy and refining sectors, where plants are expected to run for 20 years or more, accurate estimates are clearly hard to obtain (Fichtner et al., 2002; Schwaderer, 2012). Therefore, the ROI is widely used for technology assessments (Mansoornejad et al., 2010; Schaidle et al., 2011; Sen et al., 2012), and even profit calculations may sometimes be useful (Ekşioğlu et al., 2015; Liu and Pistikopoulos, 2008). Thus, for our technology assessments, we used capacity optimization models based on profit or ROI maximization as the starting point for applying our nonlinear optimization approach.

In the following explanations and definitions, as well as in the remainder of this paper, we use the indices, variables and parameters shown in Table 1.

Table 1: Model indices, variables and parameters

Fixed configuration	Variable configuration	Description	Unit of Measurement
Indices			
$i \in I$		Primary refining processes	
$j \in J$		Secondary refining processes	
$q \in Q$		Intermediate substances	
Variables			
x	x_i	Capacity of the plant/process i	$t_{products}$/yr
	m_q	Mass of intermediate substance q that is combusted (slack variable)	$t_{products}$/yr
Parameters			
p_p	$p_{p,j}$	Product price	€/$t_{products}$
a	a_i,a_j	Specific investment values	€/($t_{products}$yr)
δ	δ_i, δ_j	Cost-capacity exponents	
	s_q	Share of intermediate substance q in the stream from primary refining	
	$s_{q,j}$	Share of intermediate substance q in the product stream of process j	%
p_e		Electricity price	€/$t_{products}$
c_b		Biomass cost at plant gate	€/$t_{biomass}$
Θ		Biomass-to-products ratio	$t_{biomass}$/$t_{products}$
c_{ft}		Fixed transportation cost	€/$t_{biomass}$
c_{vt}		Variable transportation cost	€/($t_{biomass}$km)
φ		Factor for investment-related cost	%
Ψ		Biomass availability	$t_{biomass}$/(km^{2}yr)
k		Plant electricity demand	% (of product mass)

1.2.1 Approach for biomass conversion plants with a fixed configuration

To determine whether a biomass conversion plant can be competitive on the basis of price estimations for biomass and oil, one must approximate the development of all decision-relevant cost parameters relative to capacity *x*. The costs of operating a biomass conversion plant can be sub-divided into costs for biomass, electricity and investments. The latter includes several smaller cost items that can be approximated as a percentage of the expected investment (Towler and Sinnott, 2013; Vogel et al., 2008).

Biomass costs “at the plant gate” are often used to calculate input material costs (Vogel et al., 2008; Wright et al., 2008). However, because the specific biomass transportation costs (i.e. per ton of biomass that is transported) increase with capacity, this simplification becomes inaccurate when capacities are variable. Therefore, we divide biomass-related costs into biomass purchasing costs at the point of origin, distance-fixed transportation costs and distance-variable transportation costs. Both biomass purchasing costs and distance-fixed costs are assumed to rise linearly with plant capacity. However, as mentioned earlier, distance-variable costs are best approximated by a factor containing the plant capacity to the power of 1.5 (Lauven, 2014; Wright and Brown, 2007), which leads to non-linearity. When the plant capacity is expressed in tons of output produced per year, the biomass-to-products ratio Θ [$t_{biomass}/t_{products}$] can be used to determine the corresponding required quantity of biomass input. The approximation of the transportation distance depends on the average yield of suitable biomass in the surrounding area. A factor for biomass availability, Ψ [$t_{biomass}/km^2yr$], can be used to approximate biomass-related costs for a plant capacity *x*.

Several elements of investment-related costs can be expressed as a percentage of the estimated investment (Peters et al., 2003; Schwaderer, 2012; Towler and Sinnott, 2013). These ancillary costs are added up to obtain a single factor, φ (Haase, 2011). The investment-related cost factor φ is calculated as the sum of values for depreciation, operating cost (excluding input materials) and minimum ROI. The investment-related cost for a biomass conversion plant can then be calculated using an economies of scale approach. For a general investigation, a cost-capacity exponent $\delta \in (0,1)$ is used. The parameter *a* denotes the investment for a plant capacity of 1 t/yr. This approach is typical for economy of scale calculations and makes it possible to express the prospective investment as a function of capacity (Towler and Sinnott, 2013). The investment-related cost ($c_{Investment\text{-}related}$) for a plant with capacity *x* can therefore be approximated by

$$c_{Investment-related} = \varphi a x^{\delta}. \tag{1}$$

When subtracted from product sales, these cost items can be used to calculate either of the following two objective functions: profit maximization, $g_P(x)$; and ROI maximization, $g_{ROI}(x)$. Although ROI calculations are more relevant for investment decisions (Peters et al., 2003), we also discuss profits to show how the investment term in the denominator of the ROI influences the determination of optimal variable values.

$$\max g_P(x) = \\ x p_p - \varphi \mathrm{a} x^{\delta} - \theta\left(c_b + c_{ft}\right)x - \frac{c_{vt}\theta^{1.5}}{\sqrt{\pi \cdot \Psi}} x^{1.5} - p_e \mathrm{kx} \tag{2}$$

$$\max g_{ROI}(x) = \\ \frac{g_P(x)}{\mathrm{a}x^{\delta}} \tag{3}$$

The objective functions are modeled with nonlinearities for the economies of scale and variable transportation costs. The two nonlinear terms in the objective functions affect their general shapes in different ways; the term for variable transportation costs is concave, whereas the term for investment-related costs is convex--assuming typical cost-capacity exponents in the range of 0.6 to 0.8 (Peters et al., 2003). This makes the resulting sum hard to solve (Teksan and Geunes, 2015). Because the relative size of these two terms depends on the case-specific parameter values, it is impossible to make any generalized statement about the shape of the function. Instead, each application of the model must be examined separately, that is, with its case-specific parameter values.

The inclusion of a minimum ROI value in the investment-related cost factor φ can help to approach this problem at a break-even price level. Such break-even prices are generally calculated for new technologies to gain an understanding of how much a technology's economics need to improve to become competitive in the existing market environment (Nykamp et al., 2014). If the prices of hydrocarbon products are considered functions of the price of mineral oil, then the break-even oil price can be understood as the price needed to cover all costs including a minimum ROI. At the break-even price, profit maximization will determine that the required minimum ROI can be earned, but no further profits are made. If ROI maximization is used instead, the result is the same: the optimal plant configuration leads to an additional ROI of zero, but the required minimum ROI is earned. The profit maximization objective function has a degree of 1.5 due to the biomass transportation costs. In contrast, the ROI function only has a grade of approximately 0.8, since the transportation costs are divided by an investment term that usually features a cost-capacity exponent of around 0.7. Because the functions' grades and shapes differ from each other, there are two equivalent ways to determine the optimal capacity value, as the following equations show. If

$$max\, g_P(x^*) = 0, \tag{4}$$

then

$$g_P(x) \leq 0 \; \forall \; x > 0. \tag{5}$$

Because the only difference between the two functions is that in $g_{ROI}(x)$, $g_P(x)$ is divided by x^δ , given that $a > 0$ and $x > 0$, this also means that

$$g_{ROI}(x) = \frac{g_P(x)}{\mathrm{a}x^\delta} \leq 0 \; \forall \; x > 0. \tag{6}$$

And, therefore, that

$$max\, g_{ROI}(x) = 0. \tag{7}$$

Accordingly, the maximum of $g_{ROI}(x)$ is also zero at the same optimal capacity x^*, as

$$g_{ROI}(x^*) = \frac{g_P(x^*)}{\mathrm{a}(x^*)^\delta} = \frac{0}{\mathrm{a}(x^*)^\delta} = 0. \tag{8}$$

The break-even oil price therefore leads to the desired equivalence of profit and ROI maximization in terms of optimal capacity determination, since Equations (2) and (3) both contain a minimum ROI value as part of the factor φ. Therefore, both Equation (2) and (3) lead to the same optimal plant capacity, provided the parameters (e.g., product prices) are chosen to yield an objective function value of zero.

In each case, a sensitivity analysis can then be performed by applying the Envelope Theorem (Sydsæter and Hammond, 2006). This theorem states that, for parametric functions, it is possible to determine the optimal variable value x^* as a function of its parameters and to treat one or several parameters as variables in order to investigate their impact on the optimal variable value x^*. Plotting the function x^* over varying parameter values therefore illustrates the impact of changes in each parameter on the optimal capacity. To analytically determine an optimal value, the first derivative of the objective functions $g_{ROI}(x)$ and $g_P(x)$ is set to zero.

$$g'_P(x) = p_p - \theta\left(c_{ft} + c_b\right) - kp_e - \delta\varphi a x^{(\delta-1)} - \frac{1.5c_{vt}\theta^{1.5}}{\sqrt{\pi\Psi}} x^{\frac{1}{2}} = 0 \tag{9}$$

$$g'_{ROI}(x) = (1-\delta)\frac{p_p - \theta\left(c_{ft} + c_b\right) - kp_e}{a} x^{-\delta} - (1.5-\delta)\frac{c_{vt}\theta^{1.5}}{a\sqrt{\pi\Psi}} x^{-(0.5-\delta)} = 0 \tag{10}$$

Solving Equation (10), it is possible to derive a term of limited complexity for the optimal capacity $x_{ROI}{}^*$:

$$x_{ROI}{}^* = \frac{(1-\delta)^2\pi\Psi\left(p_p - \theta\left(c_{ft} + c_b\right) - kp_e\right)^2}{(1.5-\delta)^2 c_{vt}{}^2\theta^3}. \tag{11}$$

This expression can be used as a general approximation of optimal capacities for biomass conversion plants, provided sufficiently accurate estimates are made for parameter values and the coefficients of the objective function. Equation (11) reveals that two parameters contained in the objective function are not found in the optimal capacity term: investment-related costs, φ, and the specific investment value, a. Because our template for the objective function was the ROI - in which profit and cost components are divided by the estimated investment - all parameters related to the estimated investment appear in both numerator and denominator. These parameters do affect the objective function value $g(x^*)$, but they do not affect the optimal capacity x^*. The influence of other parameters can be visualized by applying the Envelope Theorem, i.e. making each of them in turn the variable of Equation (11). The fixed configuration approach described thus far helps in analyzing the importance of several parameters and, therefore, in assessing the feasibility of potential biomass conversion plant investment projects. It does not, however, help to determine which biomass conversion concept is the best fit for a particular planning situation. While this question could be answered by comparing the ROI values of several potentially suitable technologies for a given site, more complex plants such as biorefineries require an integrated planning of capacity and configuration.

1.2.2 Extension for biorefineries with a variable configuration

The choice of plant capacity significantly affects the competitiveness of any biomass conversion process, but it is especially important for biorefineries. As with production facilities in the chemical or pharmaceutical industries, substances usually undergo a series of chemical or physical transformations before the final products are produced (Kallrath, 2002; Neumann et al., 2002).

The sum of the product masses for all outputs from the secondary refining section equals the plant capacity, as measured in tons of product. For biorefinery concepts in which all outputs can be used economically in several different ways (e.g., by burning them for heat or to generate electricity), the sum of the products would be proportional to the quantity of input biomass. Thus, it would constitute a feasible measure of capacity, regardless of the type of biorefinery being investigated. If there were non-marketable outputs, that is, if only a part of the intermediate chemical stream could be converted into marketable products, these would have to be included into such a sum—e.g. with negative prices to reflect their disposal costs.

In biorefineries, where there are a large number of conversion processes, intermediate product streams and final products, several problems must be solved simultaneously to determine the optimal configuration (Heffels et al., 2014; Trippe et al., 2013). To optimize biorefinery configurations, models with individual variables for the capacities of potential secondary refining processes can be implemented. In this way, one can account for the fact that some biorefinery processes yield higher-value products than others, but at higher investments. Thus, the optimization model for integrated biorefinery capacity and configuration planning should simultaneously consider the value of the products in the potential secondary refining processes and the corresponding costs, instead of assuming the range of products to be fixed.

To apply an integrated capacity and configuration planning approach, a vector of process capacities x_i must be used instead of a single variable x, as for fixed configurations. This vector represents a combination of secondary refining processes to convert a given set of biorefinery intermediate products from primary refining into final marketable products. The plant capacity as a whole is expressed as the sum of all selected processes that yield final products, $\sum_{j=1}^{n} x_j$, where x_j is the process capacity of process i in tons of products per year. In contrast to these process capacities x_1 through x_n, the capacities of the m processes that lead to the production of intermediates are labelled x_{n+1} through x_{n+m}. As with the approach that uses one optimization variable, either profit or ROI maximization may be used to determine an optimal capacity. In analogy to Equations (2) and (3), the objective functions of the multi-process model, $G_P(x)$ (12) and $G_{ROI}(x)$ (13), consist of the following components:

$$\begin{aligned}\max G_P(x) = \\ \sum_{j=1}^{n}\left(x_j p_{p,j}\right) - \varphi\left(\sum_{i=1}^{|I|}\left(a_i\left(\sum_{j=1}^{n} x_j\right)^{\delta_i}\right) - \sum_{j=1}^{n+m}\left({x_j}^{\delta_j} a_j\right)\right) \\ -\left(\theta\left(c_b + c_{ft}\right) + p_e \mathrm{k}\right)\sum_{j=1}^{n} x_j - c_{vt}\frac{\theta^{1.5}}{\sqrt{\pi \cdot \Psi}}\left(\sum_{j=1}^{n} x_j\right)^{1.5}\end{aligned} \tag{12}$$

$$\begin{aligned}\text{and } \max G_{ROI}(x) = \\ \frac{G_P(x)}{\sum_{i=1}^{|I|}\left(a_i\left(\sum_{j=1}^{n} x_j\right)^{\delta_i}\right) + \sum_{j=1}^{n+m}\left({x_j}^{\mathrm{j}} a_j\right)}.\end{aligned} \tag{13}$$

The profit function, $G_P(x)$, includes the revenue from selling the products x_j at price $p_{p,j}$ in the first sum. The second part of the function reflects the investment-related costs for both the |I| primary and the $|J|=n+m$ secondary refining processes. Fixed costs for biomass, transportation, and electricity are included in the third summand, whereas the variable costs for transportation are summed up in the last part of the objective function.

Constraints are used to ensure valid mass or molar balances (Liu and Pistikopoulos, 2008; Penkuhn et al., 1997), that is, to reflect that the available quantity of any substance is limited by both the biorefinery's overall capacity and the demand of other processes for the substance in question. Implementing mass balance constraints ensures that the mass of an intermediate substance *q* required for combustion (m_q) or upgrading ($x_{j,q}$) on the left-hand side of the equations equals the amount of that substance provided in the synthesis reaction (s_q) or in intermediate process *j* ($s_{q,j}$) on the right-hand side.

$$m_q + x_{j,q} = s_q \sum_{j=1}^{n} (x_j) + \sum_{j=n+1}^{n+m} (s_{q,j} x_j) \tag{14}$$

To make a statement about the ability of various solvers to reliably solve such a capacity and configuration optimization problem requires testing for convexity and concavity. All constraints of the optimization problem can be written as linear inequalities defining convex half-spaces. Thus, the feasible region, as an intersection of convex sets, is convex itself (Ruszczyński, 2006). If several feasible solutions are known, convexity can be investigated using the following approach: The function is neither convex nor concave if neither the inequality for testing convexity (15) nor the inequality for testing concavity (16) hold true for all α in [0,1] and for all feasible *x and y* (Ruszczyński, 2006).

$$f(\alpha x + (1-\alpha)y) \leq \alpha f(x) + (1-\alpha) f(y) \tag{15}$$

$$f(\alpha x + (1-\alpha)y) \geq \alpha f(x) + (1-\alpha) f(y) \tag{16}$$

If neither convexity nor concavity can be established, methods for convex optimization cannot reliably identify global optima. Instead, one can either apply a nonlinear solver that claims to find the global optimum even for nonconvex problems (Tawarmalani and Sahinidis, 2002) or attempt a piecewise analysis of the functions in question (Lu et al., 2014).

1.3 Application and Results

In this section, we apply the developed model to the planning of a synthesis gas biorefinery in Germany. Synthesis gas biorefineries usually consist of a synthesis gas generation section (primary refining) and a Fischer-Tropsch, methanol or dimethyl ether (DME) synthesis (secondary refining) (Boerrigter, 2006; Trippe et al., 2013). The fixed biorefinery configuration optimization model (as described in Section 1.2.1) is compared to a variable configuration model (as described in Section 1.2.2) for the same kind of facility.

1.3.1 Application data

The biorefinery capacity planning problem is modeled twice, to investigate whether the capacities determined with the fixed configuration actually warrant changes in that configuration. Because the synthesis gas biorefinery requires residual biomass (such as residual wood and straw), the parameter values listed in Table 2 are applied to both the fixed and variable configuration approaches.

Table 2: Values for general process and logistics variables

Parameter	Description	Default value
p_i	Prices	(see Table 3)
Θ	Biomass-to-products ratio	6.25 $t_{biomass}/t_{products}$ [1,2]
c_{ft}	Fixed transportation cost	3.69 €/t [1,2]
c_{vt}	Variable transportation cost	0.25 €/tkm [1,2]
φ	Factor for investment-related cost	0.25 [3,4,5]
Ψ	Biomass availability	84 t/km²yr [6]
k	Plant electricity demand	5.11% of total heating value [7]

Several references indicate an average [1](Kerdoncuff, 2008),[2](Wright et al., 2008),[3](Derouane, 2005),[4](Swain et al., 2011),[5](Vogel et al., 2008),[6](Leible et al., 2007), [7](Kreutz et al., 2008)

The value for the biomass availability factor Ψ (84 $t_{biomass}$/km²yr) is calculated from residual wood and straw figures for all of Germany (Leible et al., 2007), but very similar values were reported for regional investigations in the German states of Baden-Württemberg (Leible et al., 2005) and Lower Saxony (Walther et al., 2012). Investment-related cost items for plants that consist of biomass gasification and Fischer-Tropsch synthesis amount to around 10% of the estimated investment for various items of operating costs, 10% for capital costs and 5% for linear depreciation over 20 years. Similar assumptions were made in (Derouane, 2005; Swain et al., 2011; Vogel et al., 2008).

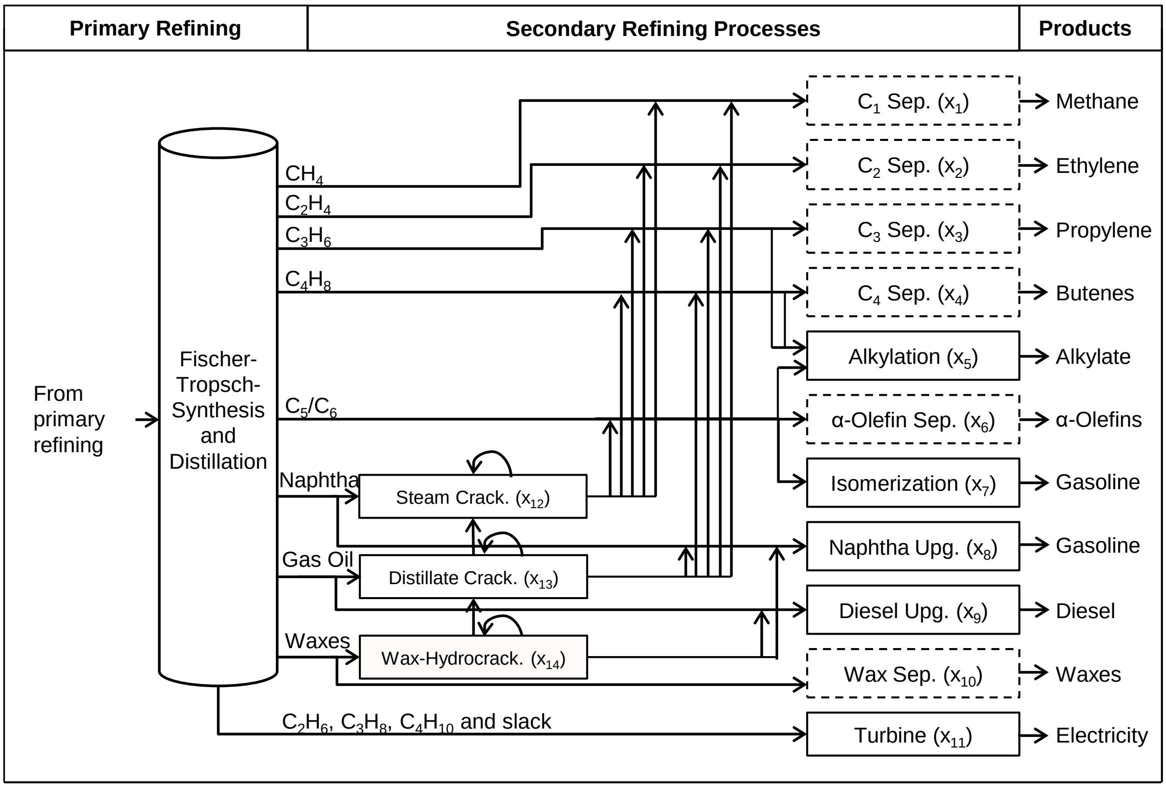

Figure 2: Potential Fischer-Tropsch upgrading and separation (dashed lines) processes

The model of a biorefinery based on synthesis gas generation from biomass focuses on the final product upgrading and separation section, which can consist of up to fourteen secondary refining processes (see Figure 2). The decision variables represent the production capacities (in t/yr) of the fourteen processes.

The Fischer-Tropsch synthesis products can be divided into eleven groups (Dry, 2004; Lauven, 2014). As shown on the right-hand side of Figure 2, eight of these product groups (methane, ethylene, propylene, the C_4 fraction, α-olefins, gasoline, diesel and waxes) are also considered final products, along with alkylate and electricity, which can be produced from several inputs. The three other original synthesis products (ethane, propane and butane) are assigned to combustion in the turbine (x_{11}) to help cover the plant's electricity consumption.

To assess the competitiveness of biorefineries having multiple products, we need forecasts of each product price. Because biorefineries compete with products made from crude oil, we approximate the competitiveness of a set of biorefinery products by means of the corresponding prices of fossil alternatives, as calculated from a break-even oil price. As described in Section 1.2, using break-even oil prices ensures that profit maximization and ROI maximization (both including a minimum ROI) have an optimal objective function value of zero at the identical optimal capacity. Product prices are calculated as the price of crude oil plus an individual product premium, which is approximated from available market data (ICIS Pricing, 2011). Table 3 shows the approximated individual product prices, both as observed in the market in the past and as estimated based on an oil price of $212/bbl, the lowest product price level at which the model returns positive objective function values. The prices for electricity and natural gas (methane) were assumed to not directly depend on the price of mineral oil.

Table 3: Products and the assumed prices at an oil price level of 212 $/bbl

Product	Assumed price at 212 $/bbl	Prices @ 80.67 $/bbl[a]	Abbreviation
Biomass	54 €/t[b]	(input)	
Electricity	185 €/t[c]	(not dependent)	
Methane	350 €/t[d]	(not dependent)	CH_4
Alkylate	1358 €/t	656 €/t	Alkyl
Ethylene	1652 €/t	950 €/t	C_2H_4
Propylene	1622 €/t	920 €/t	C_3H_6
C_4 fraction	1201 €/t[e]	682 €/t[d]	C_4H_8
C_5/C_6 α-olefins	1369 €/t	667 €/t	C_5/C_6
Naphtha	1230 €/t	528 €/t	Naph.
Diesel	1209 €/t	507 €/t	Diesel
Waxes	1944 €/t	1242 €/t	Waxes
weighted average	1203 €/t	(not applicable)	

[a](ICIS Pricing, 2011) [b](Leible et al., 2007) [c]equivalent to 35 €/MWh (European Energy Exchange, 2014), [d]equivalent to 7006 €/TJ (BAFA, 2016), [e]74% of propylene price (Peters et al., 2003)

While Figure 2 shows the processes, their inputs and outputs, Table 4 summarizes the associated investment values, the cost-capacity exponents, the variable designations in the model and, in the last row, the average values utilized in the fixed plant configuration approach. In this application, the fixed configuration uses the plant configuration of the optimal variable solution, as determined by the optimization algorithms. Accordingly, the optimization can be performed with one optimization variable representing the total plant capacity, that is, with a single economy of scale calculation, a single cost-capacity exponent and a single (average) product value (see the last lines in Table 3 and Table 4). The weighted averages were determined by calculating the required investments for both the optimal solution and a significantly smaller plant with an identical configuration.

Table 4: Processes, investment values and variable designations

Process	Investment 1 $t_{products}$/y (€$_{2015}$)	Cost-capacity exponent	Variable in the model
Methane sep.	320 [1]	0.7 [2]	x_1
Ethylene sep.	64,189 [3]	0.6 [4]	x_2
Propylene sep.	61,144 [3]	0.6 [4]	x_3
C_4 sep.	22,595 [3]	0.6 [4]	x_4
Alkylation	56,089 [1,3]	0.67 [3]	x_5
α-olefin sep.	245,679 [4]	0.6 [4]	x_6
Isomerization	4,201 [1]	0.62 [2]	x_7
Naphtha upgr.	18,160 [1]	0.625 [2]	x_8
Distillate upgr.	7,473 [1]	0.6 [2]	x_9
Wax sep.	29,825 [3]	0.67 [2]	x_{10}
Turbine	3,553 [1,2]	0.75 [2]	x_{11}
Naphtha crack.	2,518 [3]	0.7 [3]	x_{12}
Distillate crack.	2,518 [3]	0.7 [3]	x_{13}
Wax crack.	23,748 [1]	0.55 [2]	x_{14}
Biomass drying	2,259 [1]	0.77 [2]	[a]
Air Separation Unit	15,688 [2,5,6]	0.75 [6]	[a]
Gasification	27,410 [1,2,5,6]	0.67 [2]	[a]
Gas Cleaning	4,359 [1]	0.67 [2]	[a]
CO Shift	1,252 [1]	0.67 [2]	[a]
Compression	11,6557 [1]	0.67 [2]	[a]
FT synthesis	12,497 [1,2,5,6]	0.75 [2]	[a]
Product recovery	483 [1]	0.7 [2]	[a]
weighted average	138,071	0.708	x (fixed config.)

sep. = separation, upgr.=upgrading, crack=cracking, [a]primary refining process, calculated from total plant capacity (no decision variable), several references indicate that an average is used, [1](Bechtel, 1998), [2](Kreutz et al., 2008), [3](Peters et al., 2003), [4](Towler and Sinnott, 2013), [5](Boerrigter, 2006), [6](Tijmensen et al., 2002)

This made it possible to determine a cost-capacity exponent for this plant capacity and subsequently determine a value for the required investment. Using the fixed configuration approach, the average break-even product value was determined (see the last row of Table 3).

The investment values for both primary and secondary refining processes shown in Table 4 were found in several reports on the feasibility of biofuel production via synthesis gas that were published from the late 1990s onwards (Bechtel, 1998; Boerrigter, 2006; Kreutz et al., 2008; Tijmensen et al., 2002). Because chemical separation and upgrading was not usually included in these so-called Biomass-to-Liquid designs, the chemical separation units were calculated from values found in general chemical engineering literature (Peters et al., 2003; Towler and Sinnott, 2013). All investment values were adjusted to 2016 prices using the German Chemie-Ingenieur-Technik index, also known as Kölbel-Schulze index, since it is the prevalent plant construction index for Germany (VCI, 2016). Because most of the original investment data referred to plants in the United States, the US$ values were converted to Euro (before 2002, to German Mark) values using the currency exchange rate of 1994. This was the reference year of (Bechtel, 1998), from whom most of the investment data was derived, and was also the basis year for (Kreutz et al., 2008), who published process-specific cost capacity exponents. Due to the uncertainty involved in combining investment data from different sources into a single model, the optimization results should be regarded merely as illustrative for our given case study.

Mass balance constraints for the substances considered in this case study are shown in Equations 17 through 24.

Methane:

$$m_{CH_4} + x_1 = s_{CH_4} \cdot \sum_{j=1}^{11} (x_j) + s_{CH_4,12} \cdot x_{12} + s_{CH_4,13} \cdot x_{13} \tag{17}$$

Ethylene:

$$m_{C_2H_4} + x_2 = s_{C_2H_4} \cdot \sum_{j=1}^{11} (x_j) + s_{C_2H_4,12} \cdot x_{12} + s_{C_2H_4,13} \cdot x_{13} \tag{18}$$

Propylene:

$$m_{C_3H_6} + 0.4 \cdot \frac{s_{C_3H_6}}{s_{C_3H_6} + s_{C_4H_8}} \cdot x_5 + x_3 = s_{C_3H_6} \cdot \sum_{j=1}^{11} (x_j) + s_{C_3H_6,12} \cdot x_{12} + s_{C_3H_6,13} \cdot x_{13} \tag{19}$$

Butenes:

$$m_{C_4H_8} + 0.4 \cdot \frac{s_{C_4H_8}}{s_{C_3H_6} + s_{C_4H_8}} \cdot x_5 + x_4 = s_{C_4H_8} \cdot \sum_{j=1}^{11} (x_j) + s_{C_4H_8,12} \cdot x_{12} + s_{C_4H_8,13} \cdot x_{13} \tag{20}$$

C_5 and C_6 hydrocarbons:

$$m_{C_5/C_6} + x_6 + x_7 + 0.6 \cdot x_5 = s_{C_5/C_6} \cdot \sum_{j=1}^{11} (x_j) + s_{C_5/C_6,12} \cdot x_{12} \tag{21}$$

Gasoline range hydrocarbons:

$$m_{Naph.} + x_8 + x_{12} = s_{Naph.} \cdot \sum_{j=1}^{11} (x_j) + s_{Naph.,12} \cdot x_{12} + s_{Naph.,13} \cdot x_{13} + s_{Naph.,14} \cdot x_{14} \tag{22}$$

Diesel range hydrocarbons:

$$m_{Diesel} + x_9 + x_{13} = s_{Diesel} \cdot \sum_{j=1}^{11} (x_j) + s_{Diesel,14} \cdot x_{14} \tag{23}$$

Wax range hydrocarbons:

$$m_{Waxes} + x_{10} + x_{14} = s_{Waxes} \cdot \sum_{j=1}^{11} (x_j) \tag{24}$$

Although these constraints ensure the validity of the underlying mass balances, additional constraints are required to represent the technical characteristics of several upgrading processes, which either utilize only a part of a product stream (in case of the α–olefin separation capacity, x_6) or several streams at the same time (in case of alkylation capacity, x_5). A detailed description of these processes can be found in (Lauven, 2014).

1.3.2 Results for a biorefinery with a fixed configuration

For the fixed configuration approach introduced in Section 1.2.1, the graphs of the profit and ROI functions are shown in Figure 3. Because we assumed that Θ = 6.25 tons of residual wood and straw are required to produce a ton of hydrocarbon product (see Table 2), the values for a plant capacity x would have to be multiplied by this factor Θ to determine the required biomass input. The objective function for profit maximization, $g_P(x)$, falls steeply for low capacities, before starting to rise for capacities above 200,000 tons per year. From this point onwards, investment-related cost reductions overcompensate the increasing biomass transportation costs.

After both functions reach a maximum at around 1.6 million tons of products per year, this development is reversed. In contrast to the objective function for profit maximization, $g_P(x)$, the ROI objective function $g_{ROI}(x)$ is concave, which indicates that there is a (global) maximum at approximately 1,634,000 tons of products per year. This corresponds to an input of more than 10 million tons of residual biomass per year, which would require some 30% of the straw and residual wood available annually in Germany (Leible et al., 2007). Moreover, $g_{ROI}(x)$ rises steeply for very low capacities, but changes very little for a very broad range of capacities in excess of around 500,000 tons of products per year, that is, for inputs of 3,125,000 tons of residual biomass, or more. Thus, while the profit function is very sensitive to changes in capacity, this sensitivity is significantly reduced if the required investment is taken into account, as in ROI calculations.

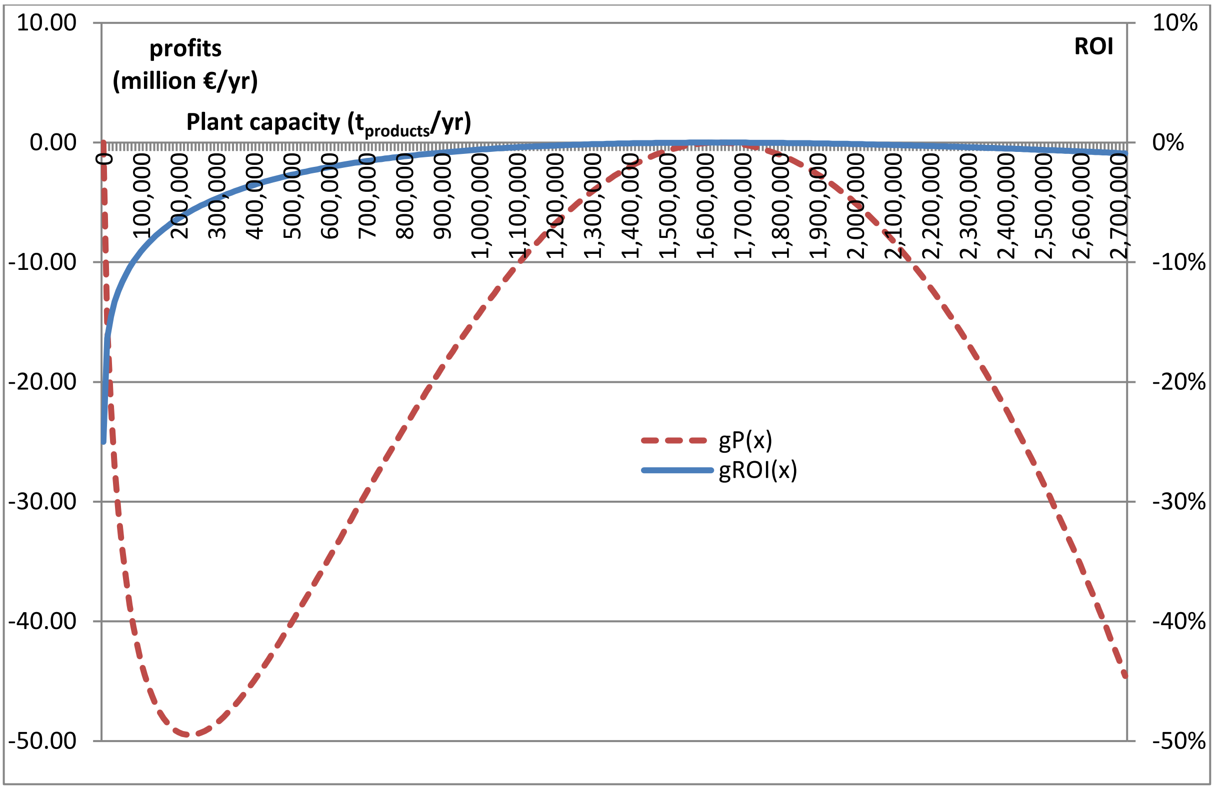

Figure 3: Shape of the objective functions for profit, $g_P(x)$ (dashed line), and ROI, $g_{ROI}(x)$, maximization

When comparing capacity optimization approaches, one should remember that ROI optimization generally leads to lower optimal capacities than profit optimization, since the profit term (which is identical for both functions) is divided by the required investment for the ROI calculation (Peters et al., 2003). Rising profits due to larger capacities therefore always lead to a higher objective function value for profit maximization, but not necessarily to a higher ROI; for ROI, a rise in profits may be overcompensated by the corresponding rise in the required investment. Summing up, profit-based determinations of optimal capacity are likely to overestimate both the optimal capacity and its impact on the competitiveness of the investment. Because the ROI is the more meaningful indicator for investment decisions (Peters et al., 2003), the profit-based capacity optimization should be viewed cautiously in any case.

To supplement the insights provided by Figure 3, a sensitivity analysis can be carried out using the Envelope Theorem. This fosters a general understanding of the impact of the objective function's parameters, as described in Section 1.2.1. Figure 4 shows that the optimal capacity increases with rising product prices and biomass availability and decreases for a rising conversion ratio of the biorefinery, the variable transportation cost and biomass prices. Changes in biomass availability result in linear changes in the optimal plant capacity. The corresponding reaction to changes in the biomass price is nonlinear, but the deviation from a linear relationship is rather small. For increasing product prices and decreasing conversion ratios or variable transportation costs, the capacity is visibly nonlinear and more than doubles for parameter changes of less than 50%. The sensitivity analysis thus indicates that research directed at improving the conversion efficiency of the plant would be a promising way to achieve larger capacities, since it would improve the conversion ratio. It should be noted that favorable changes, that is, rising product prices and falling conversion ratios and variable transportation costs, also lead to significantly higher optimal plant capacities. In contrast, the impact of unfavorable changes decreases continuously with increasing deviation from the original parameter estimate (i.e., 100%).

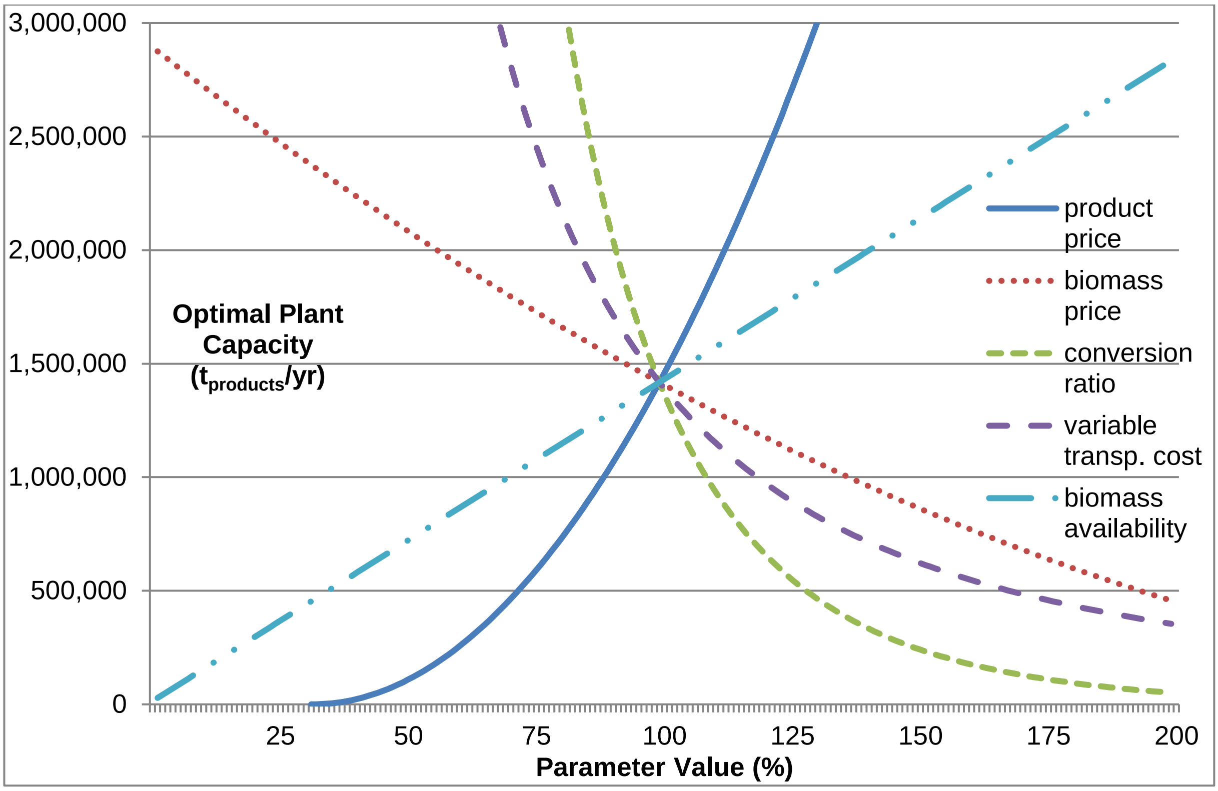

Figure 4: Envelope Theorem-based sensitivity analysis for selected parameter values between 0 and 200%

While the role of improved logistics has already received significant attention (e.g., (Kerdoncuff, 2008; Peters et al., 2003), increasing the average product value also appears to offer further potential for more competitive economics (Lauven, 2014; Trippe et al., 2013). The choice of synthesis products (e.g., Synthetic Natural Gas (SNG) vs. fuels vs. chemicals) therefore plays a major role in determining the optimal capacity, and thus, the economic competitiveness of the plant.

1.3.3 Results for a biorefinery with a variable configuration

To analyze which products would be most beneficial for the biorefinery, the plant can also be modeled with a variable configuration, as described in Section 1.2.2. The optimization problem for variable configurations has fourteen optimization variables and, coincidentally, fourteen constraints. Because finding a feasible solution may be a problem for some nonlinear programming solvers, the starting points were varied to increase the likelihood of encountering the global optimum. Drawing on an approach for investigating solver performance for MINLP problems (Jüdes et al., 2008), we included both non-feasible and feasible starting points. For the optimization, we applied five GAMS solvers for nonlinear problems: CONOPT, MINOS, SNOPT, KNITRO and BARON. We chose GAMS, a modeling editor published by the World Bank (Rutherford, 1999), because switching between solvers requires only one change to the optimization model. This made it possible to solve the capacity planning problem for the biorefinery with five different solvers and compare the solutions. This seemed advisable, since similar investigations on the use of MINLP for power plants reported regular failures of some solvers to optimally solve (mixed-integer) nonlinear problems (Jüdes et al., 2008).

The best solution found by any applied solver, labelled x^*, was only reliably identified by the BARON (Branch-And-Reduce Optimization Navigator) solver (see Table 5). The objective function ROI value of this solution is 0.189%, which leaves a theoretical optimality gap of 0.021% ROI, according to the BARON results. It was sometimes also found by the other solvers, but hardly ever from the same set of starting values or with the same objective function. x^* includes a wax upgrading unit (x_{10}) that purifies waxes for sale. If the starting values were in the order of magnitude of x^*, the CONOPT solver found this solution exclusively with the objective function for ROI maximization, while the KNITRO solver found it only with the objective function for profit maximization. SNOPT and MINOS only returned this solution if starting values identical to the optimal solution were supplied. For small starting values (1,000 and 10,000 $t_{product}$/yr for all processes), CONOPT returned a similar solution, here labelled x^+ for comparison purposes and an investigation of convexity and concavity. This solution has a slightly lower total plant capacity and objective function value (-1.26% ROI instead of +0.189%) and includes a wax hydrocracking unit (x_{14}). Both x^* and x^+ are similar to the chemical-oriented configuration used in the Secunda Coal-to-Liquid plant of the company Sasol in South Africa - a configuration that takes advantage of the chemicals produced along with the fuels in the synthesis reaction (Dancuart et al., 2006).

The total plant capacities of both solutions are in the same range as that of the fixed configuration. This is unsurprising for x^*, since its configuration is the same as that of the fixed configuration approach. The total plant capacity of x^+ is slightly smaller (some 140,000 tons of hydrocarbons per year) and due to the wax hydrocracking unit, there is more cracker capacity (x_{12}-x_{14}) in this solution. Thus, in x^+, more chemicals and fewer waxes are produced. Clearly, price estimates play a key role in determining optimal plant configurations and capacities.

The number of variables and constraints in this case study is not an obstacle for most solvers. However, since most nonlinear solvers can merely guarantee globally optimal solutions for convex or concave problems, the choice of a suitable solver is crucial.

Table 5: Solutions x^* and x^+ [$t_{products}$/yr]

Variable	Solution x^+	Solution x^*
x_1 (Methane Upgrading)	212,381	225,900
x_2 (Ethylene Separation)	269,170	279,321
x_3 (Propylene Separation)	295,972	312,586
x_4 (C_4 Separation)	204,117	214,487
x_5 (Alkylation)	0	0
x_6 (α-olefin Separation)	0	0
x_7 (Isomerization)	274,511	300,109
x_8 (Naphtha Upgrading)	125,050	94,838
x_9 (Distillate Upgrading)	0	0
x_{10} (Wax Separation)	0	87,107
x_{11} (Turbine)	122,147	129,182
x_{12} (Naphtha Cracking)	300,669	328,706
x_{13} (Distillate Cracking)	304,353	276,113
x_{14} (Wax Hydrocracking)	79,677	0
Total Plant Capacity (x_1-x_{11})	1,503,347	1,643,533

1.4 Discussion

In planning biorefineries, one must take into account the numerous potentially beneficial products and the widely-distributed biogenous input materials. Our goal was to show that additional insights about the optimal product spectrum can be gained from an integrated capacity and technology-choice model. To highlight the benefits of this integrated planning approach, we compared it to an approach lacking a configuration optimization.

1.4.1 Biomass conversion plant planning

Both the fixed and the variable plant configuration approaches offer benefits for biomass conversion plant design. Whereas the fixed configuration helps approximate optimal capacities for biomass conversion plants having a pre-determined product portfolio (such as bioethanol, biodiesel or biomass CHP plants), the variable configuration approach is useful when the product spectrum itself is up for consideration. With the fixed configuration approach, trade-offs between smaller and larger plants can be examined to determine optimal capacities much more accurately than existing rules of thumb allow. For example, instead of assuming a fixed maximum transportation distance of 30 or 50 km, transportation costs and investment-related costs can be treated as functions of plant and process capacities. Therefore, insights gained through the fixed configuration modeling approach (e.g., the equation for determining optimal plant capacities for fixed configuration plants, Equation (11)), can be used to deliver a good estimation of capacity intervals, which in turn allows for more detailed plant and equipment planning.

The plant capacities determined in the case study are much larger than those of existing biomass conversion plants. Both modeling approaches lead to optimal plant capacities of more than 1.6 million tons of hydrocarbon products per year. This is significantly larger than many capacities discussed in existing literature, with the exception of (Boerrigter, 2006). Although the optimization results suggest that the influence of biomass transportation costs may have sometimes been overestimated in planning processes, biomass procurement does become more difficult and more risky for large biorefineries.

Because numerous competing biomass users must be expected in densely inhabited countries like Germany, the application of such models could become interesting for plants being planned in parts of the world where biomass is not such a highly sought-after commodity.

The optimal configuration determined with the variable configuration approach, which focuses on chemicals production, differs significantly from the liquid fuels configurations discussed in literature. Given that the assumed premium-based calculation of product prices realistically approximates product prices, the higher value of chemicals appears to justify additional investments in some separation processes at oil prices above $200/bbl.

If oil prices were to reach such levels, biomass prices would however likely be affected as well. Using break-even oil prices to assess the economic feasibility of biomass conversion concepts therefore means that interactions between oil and biomass prices, as described in (Nordhoff et al., 2007), should also be considered in future research. Since the determined break-even oil prices are roughly four times higher than the actual 2017 prices, such a synthesis gas biorefinery is unlikely to be realized at this time. Nevertheless, the future development of biomass and output prices is likely to make biorefinery configuration and capacity planning necessary for some types of biorefineries. Because the associated planning process may use the same modeling approach but require different parameter values, we will discuss the implications of using the presented nonlinear approach in the next sub-section.

1.4.2 The nonlinear modeling approach

Reliably solving a nonlinear optimization problem requires knowledge about the shape of the investigated functions. In order to assess whether the problem at hand is convex, concave or neither, we use two solutions x^* and x^+, which are both part of the feasible region. We can verify the non-convexity and non-concavity of both objective functions for variable configurations--profit maximization $G_P(x)$ and ROI maximization $G_{ROI}(x)$--since the following tests for non-convexity and non-concavity (Equations 25 through 28) hold true:

$$G_P(0.5x^* + 0.5x^+) \leq 0.5G_P(x^*) + 0.5G_P(x^+) \tag{25}$$

$$G_P(0.5 \cdot 0.99x^* + 0.5x^*) \geq 0.5G_P(0.99x^*) + 0.5G_P(x^*) \tag{26}$$

$$G_{ROI}(0.5x^* + 0.5x^+) \leq 0.5G_{ROI}(x^*) + 0.5G_{ROI}(x^+) \tag{27}$$

$$G_{ROI}(0.5 \cdot 0.99x^* + 0.5x^*) \geq 0.5G_{ROI}(0.99x^*) + 0.5G_{ROI}(x^*) \tag{28}$$

Because ROI maximization (Equation (3)) is a concave function, the capacity-planning problem with fixed configuration can be solved to optimality. However, including all fourteen separation and upgrading processes in the optimization problem alters the objective function, resulting in a general nonlinear optimization problem with an objective function that is neither convex nor concave. Therefore, standard convex optimization methods no longer yield optimal solutions in every instance (Simmons, 1975). Nor can special approaches for optimizing concave functions over a convex set (Horst, 1984) be used. This non-convexity is caused by the additional variables representing the additional capacities for specific products. Due to the non-convex and non-concave nature of the presented problem, only algorithms designed for non-convex optimization are suitable for solving the described integrated configuration and capacity-planning problem.

Among the applied solvers, only BARON is a nonlinear solver that can yield optimal values in non-convex or non-concave nonlinear problems. It is a Branch-and-Bound algorithm for nonlinear global optimization that employs various pre-processing and post-processing steps for bound improvement (reduction). The bounding scheme of the algorithm is consistent, that is, any unfathomed sub-problem in the decision tree can be further refined, and the upper and lower bounds will eventually converge for any sequence of decreasing partitioning of the sub-problem. The algorithm's selection scheme is bound improving, which means that the sub-problem with the lowest bound will eventually be chosen for further investigation after a finite number of steps (Tawarmalani and Sahinidis, 2002). Horst and Tuy, (1996) have shown that any branch and bound algorithm for continuous optimization problems will eventually converge under these conditions. Therefore, the BARON solver is able to solve non-convex nonlinear problems to optimality. Our results indicate that, due to the irregular shape of the objective function, the other investigated solvers do not always identify the optimal solution x^*, yet often converge to other local optima. Only with the BARON solver can we confirm that x^* is indeed the optimal solution.

Piecewise linearization, which is customary in refinery scheduling or gas network problems (Fügenschuh et al., 2014; Gao et al., 2015), is another way to approximate a solution for non-convex problems. It was not investigated in this case, since the number of nonlinear terms and optimization variables in the investigated optimization problems may lead to increasing inaccuracies and significant additional efforts (Penkuhn et al., 1997). This is due in part to the fact that the number of simplices required for the piecewise linearization increases drastically with the dimension of the nonlinear optimization problem (Geißler et al., 2012). Moreover, the extra efforts required with piecewise linearization are usually problem-specific and hence, non-transferrable. In contrast, using a direct nonlinear optimization approach model, such as the one presented in this paper, facilitates adaption of the model to new planning situations.

1.5 Conclusion and outlook

In this paper, we present nonlinear optimization models for fixed and variable plant configurations and apply them to capacity and configuration planning for biorefineries. The model for fixed configurations (Section 1.3.2) shows how an analytical approach can quantify the influence of decisive parameters for biomass conversion plant investments. With this model, one can approximate optimal capacities from a limited number of process parameters and perform Envelope Theorem-based sensitivity analyses. This helps to analyze the impact of changes in individual process parameters on a technology's economic potential. The sensitivity analysis illustrates the considerable impact of changes in conversion ratio and variable transportation costs on the optimal plant capacity for the investigated scenario. It also reveals that the attainable average product value significantly affects the economic potential of a biomass conversion plant. For a plant producing either a single product or a fixed set of products, an analytical investigation can be used to illustrate the influence of certain parameters. The objective function for Return on Investment (ROI) maximization is especially suitable for this purpose. Because the plant and process capacity intervals covered are large, the results are less accurate than those of feasibility studies at a fixed capacity. Nonetheless, they may still serve as a useful first step in identifying competitive plant technologies and promising capacities. Although we determined break-even oil prices in this paper, one could also use current market prices to determine the price of CO_2 emission certificates at which biomass conversion plants become competitive with fossil fuel plants.

The integrated capacity and configuration optimization for variable configurations can consider several upgrading options as a vector of variables. This makes it possible to optimize a biorefinery configuration over continuous capacities, instead of merely comparing discrete configuration options. Thus, the integrated approach is suitable for biorefineries in which a large number of alternative products could theoretically be produced and sold. The question to be answered then is whether the added value of the higher quality products justifies the additional investment in separation equipment. Furthermore, units to produce intermediate substances can be included in the model to represent chemical reactors that increase the quantities of certain intermediates at the expense of others. The successful implementation of such conversion units in a nonlinear optimization model makes it possible to investigate further technological options and therefore contributes to a more realistic and more widely applicable techno-economic modeling in this field.

In the case study for Germany, we found the global optimum of the described nonlinear optimization problem using the BARON solver, which is designed to specifically handle nonconvex optimization; in contrast, the other four solvers failed to reliably find the optimal solution. The promising results obtained here encourage the use of more elaborate objective functions. Examples might be those functions required for dynamic methods of investment and cost estimation in the process industry--such as the net present value (NPV)--instead of the static profit or ROI functions (Kallrath, 2002).

If data on existing biomass demand can be included, then the single-product capacity optimization models can be applied to simultaneously compare a large number of potential locations for several biomass conversion technology options. Since such data is indeed available for several countries in Geographic Information Systems (GIS), GIS-based planning approaches can be used to extend the presented Operations Research models to include site selection. The variable configuration approach would then make it possible to identify the most economical biorefinery location, capacity and configuration from a nearly infinite number of potential biorefinery concepts. These would be characterized by a specific combination of input materials, conversion and upgrading technologies and products within a predefined region or country (Schröder et al., 2017). As the identification of feasible biorefinery concepts becomes easier, it stands to reason that the realization of those concepts becomes easier as well. This development should lead to more efficient utilization of scarce biomass resources, which is important in a future bioeconomy that will rely to a much higher degree on biogenous input materials (OECD, 2009).

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