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Optimization of Biomass-to-Liquid Plant Setups and Capacity Using Nonlinear Programming

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List of Abbreviations

AGEB	Arbeitsgemeinschaft Energiebilanzen
ASF	Anderson-Schulz-Flory
ASU	Air Separation Unit
bbl	Barrel
BMU	Bundesministerium für Umwelt und Naturschutz
BtL	Biomass-to-Liquid
C_{2+}	Hydrocarbons with two or more carbon atoms
CBtL	Coal-and-Biomass-to-Liquid
CEPCI	Chemical Engineering plant cost index
CNG	Compressed Natural Gas
CtL	Coal-to-Liquid
CUTEC	Clausthaler Umwelttechnik Institut
DENA	Deutsche Energie-Agentur
DFC	Distance fixed costs
DME	Dimethylether
DOE	(US) Department of Energy
DVC	Distance variable costs
DVGW	Deutscher Verein des Gas- und Wasserfachs
EEG	Gesetz für den Vorrang Erneuerbarer Energien
EnWG	Energiewirtschaftsgesetz
ETBE	Ethyl-tertiary-butyl-ether
FNR	Fachagentur Nachwachsende Rohstoffe
FT	Fischer-Tropsch
GAMS	General Algebraic Modeling System
GHG	Greenhouse gas
GtL	Gas-to-Liquid
GW_{th}	Giga-Watt (thermal)
ha	hectare
HTFT	High temperature Fischer-Tropsch
ICE	Internal combustion engine
IGCC	Integrated Gasification Combined Cycle
ILOP	Integer
IPCC	International Panel on Climate Change
KIT	Karlsruhe Institute of Technology
kWh	Kilo-Watt-hour
kWh_{el}	Kilo-Watt-hour (electric power)
kWh_{th}	Kilo-Watt-hour (thermal)
LPG	Liquid Petroleum Gas
LTFT	Low temperature Fischer-Tropsch
MADM	Multi-attribute decision making
MCDM	Multi-criteria decision making
MeOH	Methanol
MIP	Mixed Integer Program
MILP	Mixed Integer Linear Program
MJ	Mega-Joule
MODM	Multi-objective decision making
MtD	Methanol-to-Dimethylether
MtG	Methanol-to-Gasoline
MtH	Methanol-to-Hydrogen
MtO	Methanol-to-Olefins
MtP	Methanol-to-Propylene
MtPower	Methanol-to-Power
MtSynfuels	Methanol-to-Synthetic fuels
MW	Megawatt
MW_{th}	Megawatt (thermal)
NFRP	Nelson-Farrar Refinery Process (index)
NLP	Nonlinear Program
NO_X	Nitrogen Oxides
NPV	Net present value
OPEC	Organisation of Petroleum Exporting Countries
PSA	Pressure Swing Absorption
pH-value	Potencia hydrogenii
RME	Rape Seed Methyl ester
ROI	Return on Investment
RON	Research Octane Number
RSA	Republic of South Africa
SNG	Substitute Natural Gas
TWh	Terra-Watt hour

Variables declaration

a_i	specific investment for process I [€]
b_j	price of product j [€/t]
c_k	share of hydrocarbon k in the Fischer-Tropsch product distribution [%]
f_w	distance fixed transportation costs for means of transportation w [€/t]
k_y	specific costs associated with situation y [€/t]
K_y	total costs associated with situation y [€]
v_w	distance variable transportation costs for means of transportation w [$\frac{€}{t \cdot km}$]
s_k	quantity of a hydrocarbon k that is combusted [t/a]
u	share of truck transportation in combined traffic settings
α	probability of hydrocarbon chain growth in the Fischer-Tropsch synthesis
β	factor for the calculation of investment-related costs from total plant investments [€/a]
δ_i	cost-capacity exponent for process i
ε_n	constraint limits of objective n in the ε-constraint method
θ	tons of biomass required per ton of products [$\frac{t_{biomass}}{t_{products}}$]
ξ	share of hydrocarbons in the Anderson-Schulz-Flory distribution [%]
σ_n	weighting factor of objective n in the weighting method
φ	average assumed distance between two freight terminals [km]
ψ	availability of residual biomass (straw and residual wood) [$\frac{t}{km^2}$]
ω	conversion factor from variable value to process capacity [t/a]

1 Introduction

Scarce fossil energy resources, resulting in steeply rising prices, have fuelled the development of alternative concepts to supply energy and other fossil-derived products such as organic chemicals in several periods in the 20^{th} century. The economic importance of liquid hydrocarbons has been a driver of technical innovation during periods with high prices of crude oil. While other fossil resources, such as coal or natural gas, have been the preferred choice as substitutes for crude oil in the earlier disruptions of crude oil supply, developments in the final quarter of the 20^{th} century have led to a shift in attention towards renewables (Bundesregierung 2010, p. 3; BMU 2011, p. 3). Concerns about climate change, which is generally assumed to be triggered by a rising level of greenhouse gases in the atmosphere, have promoted the reducing greenhouse gas emissions resulting from the conversion of fossil energy carriers to water and carbon dioxide (IPCC 2007, p. 30). Numerous renewable sources of energy have been developed and promoted in recent decades (BMU 2011, p. 5). Processes to produce power from wind, solar radiation, geothermal energy and biomass are among the most visible developments to reduce fossil fuel consumption for power generation. While this approach is feasible to tackle the considerable portion of anthropogenic CO_2 emissions resulting from coal combustion in power plants, its effect on transportation is, as of now, limited. Until concepts independent of hydrocarbon fuels, like e-mobility, can be used to cover mobility needs, the production of liquid hydrocarbon fuels therefore remains a necessity.

If it is assumed that the supply of oil will be insufficient to cover the rising world demand or even peak at some point in the near future, oil prices are likely to rise and require the pursuit of alternatives for crude oil's areas of application (Erdmann/Zweifel 2007, p. 207). Biomass, the most versatile renewable energy, can be part of the solution to this problem. In addition to using biomass for power production via direct combustion or combustion of biogas produced by fermentation, biomass can also be used for the production of liquid transportation fuels (Kaltschmitt 2001, p. 4). Converting sugars to bioethanol, or plant oils to biodiesel, is already pursued on a large scale in many industrialized and some transition economies around the globe. Among the initial reasons to promote the use of crops from agriculture for fuel production in the technologies' earlier stages was the reoccurring situation of large agricultural surpluses in industrialized countries. By developing new paths of usage for agricultural products, these surpluses were reduced. In the European agricultural reform of 1992, 15 % of the agricultural land was legally required not to be used for food production. The only plants that could be planted and harvested on these unused lands, were renewable resources such as rape, sunflowers or miscanthus. The share of decommissioned land was reduced to 10 % in the so-called "agenda 2000", before it was lifted in 2008, as rising demand for both food and bioenergy were found to have eliminated the need for artificial supply reductions (Schönleber 2009, p. 5ff). This shows that the potential for further increases in the production of energy crops on agricultural land is limited. In addition, the ability to produce crude oil substitutes from agricultural products linked the markets for food and energy, increasing the likelihood of rising crude oil prices to affect the prices for food

(Nordhoff, et al. 2007, p. 553; Cassman/Liska 2007, p. 18). If the prices for agricultural goods in industrialized areas like the European Union increase beyond the level sustained by subsidies, the European market for agricultural goods is likely to demand more such goods from the world markets. The potential ensuing price increases for food have been subject of intense political discussion since early 2008 (WISU 2008a, WISU 2008b).

As the (BioKraftQuG 2009) requires biofuels to be make a significant contribution to substituting fossil energy carriers in the future, mineral oil companies must identify biomass sources other than agricultural areas and use them with the greatest possible efficiency. While not as easily yielding substances for immediate use as agricultural crops do, some forms of biomass can be gasified and used for the synthesis of liquid hydrocarbons using processes for the production of so-called 2nd generation biofuels, such as Fischer-Tropsch or methanol synthesis. Such kinds of biomass include residuals from both agriculture and forestry. As the whole plant can be gasified and converted to liquid hydrocarbons, the yield per hectare is usually considered to be significantly higher than for 1st generation biofuels such as bioethanol or biodiesel.

While plants for the conversion of residual biomass (or waste) to hydrocarbon fuels have already been constructed in pilot scales, a widespread application of the technology has not yet taken place (Gottschau 2006, p. 26ff). Although biomass gasification for the production of the required synthesis gas is more complex, i.e. expensive, than gasification of coal or the reforming of natural gas, several processes exist that are technically feasible to accomplish the conversion in sufficient quantities. The core hindrance for the construction of Biomass-to-Liquid (BtL) plants appears to be economic, instead of technical, in nature. Comparable coal or natural gas conversion facilities are constructed in the vicinity of coal mines or natural gas fields. Accordingly, the costs for transporting the input materials to the conversion facility are relatively low and economies of scale can be applied to improve specific production costs.

Biomass, by contrast, has to be collected over large areas, which may be owned and tilled by numerous farmers or foresters. Transportation distances, and therefore costs, grow in more than linear terms relative to capacity (Wright/Brown 2007a, p. 194f). The higher a plant's capacity, the higher its specific biomass transportation costs (e.g. in €/ton of products). Capacities in the scale of contemporary oil refineries therefore appear infeasible for Biomass-to-liquid plants due to prohibitive biomass transportation costs. In addition, the high water content of biomass makes transportation less efficient, as well as making it necessary to dry the biomass at some point before the actual conversion can take place. Therefore, if biomass is to be economically converted to hydrocarbon fuels, an optimal plant size has to be determined to make as much use of economies of scale as possible while averting unreasonable biomass transportation costs (Wright/Brown 2007a, p. 192).

Several concepts have been developed to ease this antagonism between economies of scale and rising transportation costs either by improving the specific transportation costs or the specific investment necessary for the installation of BtL plants. For a potential realization of such a plant, is it important to know which concepts appear to be the most promising with regard to improving competitiveness. The comparison of any two concepts with different cost structures can quickly become misleading in this context. Concepts with low investment requirements are more favorable at relatively low capacities, while concepts with improved logistics concepts gain attractiveness when capacities are large. Therefore, the separation of relatively valuable chemicals may not be advantageous for low plants, but become more attractive if capacities are sufficiently large. Consequently, comparisons at a given, fixed plant capacity without consideration of potential product upgrading alternatives may favor some concepts over others.

It is the aim of this thesis to develop a decision support model that takes these differences into account appropriately. The development of both economies of scale and transportation costs can be modeled on an upgrading process basis using nonlinear functions, as these mirror the actual correlation with rising plant capacities relatively accurately. Such a model can then be used to determine optimal plant capacities for each concept individually. The comparison of the relative advantage of the concepts can then be performed by comparing a representative performance indicator, such as the level of product prices required to earn a minimum return on investment.

While linear functions are sometimes used to approximate these developments in a limited range of capacities, deviations from the actual development become significant if a large range of potential plant capacities is investigated. Linearized functions are therefore less accurate in mapping the effects of rising BtL plant capacities, as deviations may significantly alter the determined optimal plant size. Additionally, approximating the relatively large number of process-individual cost-capacity exponents would result in a considerable effort. Therefore, the nonlinear character of both economies of scale and biomass transportation costs is ideally represented by the corresponding nonlinear functions (Wright/Brown 2007a, p. 195). This approach is intended to determine whether common assumptions regarding feasible BtL plant capacities can be verified and to inquire which product distribution is optimal in a given situation.

While there are numerous proposals that appear fit to improve the competitiveness of second generation biofuels, assessing their impact by individual case studies is an arduous task. It is advisable to investigate the likelihood of actual improvements before detailed investigations are attempted. This thesis aims to represent the most significant influencing factors in an optimization model. By means of mathematical optimization and parameter variation, a large number of plant setups and proposed improvements can be analyzed with relatively little effort. If the model is found to be satisfyingly accurate, it can help to identify the most promising concepts. Based on these relative findings, more detailed investigations can then follow to verify the model's results.

In order to help develop an understanding of the current energy supply situation, the second chapter is intended to give an overview over both existing processes and potential competing concepts. Therefore, some background information about the German energy supply and the expanding share of renewables is given before the processes required for the production of 2nd generation biofuels are described in detail.

As favorable economic indicators are both necessary to attract sufficient capital for the realization of plant concepts and to guarantee an economically sustainable allocation of resources, the third chapter gives an overview over available methods to determine the economic advantage of investment projects.

In the fourth chapter, the mathematical concept of optimization is described. Several optimization approaches are introduced with a focus on the nonlinear optimization algorithms needed to solve the underlying problem.

In chapter 5, the model for the determination of optimal process setups and plant sizes is set up. The objective function with its nonlinear components is introduced as well as the linear constraints that represent mass balances, technical restrictions and similar limiting factors.

Chapter 6 shows the results if this model is applied to some common process setups for the production of 2nd generation biofuels. Exclusive fuel production is contrasted with fuels and chemicals co-production as well as from the production of SNG.

In chapter 7, the model is expanded to account for improvements of the plant and logistics concept proposed in literature. These include pretreatment of biomass, combined traffic concepts, BtL plant construction adjacent to refineries and coal and biomass co-gasification.

In the last chapter, a summary of results is given and conclusions are drawn. A special emphasis is given to the discussion of the modeling results in the context of their significance for the potential realization of BtL plants in the future.

2 Use of Renewable Energies in Germany

Since the industrial revolution, fossil fuels have increasingly been extracted from coal mines, gas fields and oil rigs in Germany to increase the amount of energy available for the generation of heat, power and transportation fuels. The relative ease with which such extractions could be achieved led to a market dominance of fossil fuels over other sources of energy. The oil crises of the 1970s and other price developments have spread the assumption that fossil fuels, especially oil and gas, will not be sufficient to ensure economic energy supply in the future. Accordingly, the adaptation of industry and transportation to the worsening supply-demand relationship of crude oil and natural gas is a major challenge for Germany and other industrialized countries. In order to dampen the expected effects of rising mineral oil prices on transportation and the chemical industry, a number of processes to replace crude oil using renewable energy sources have been developed and implemented. In the following chapter, the status quo of energy supply in Germany will be outlined with special attention on the use of renewables.

2.1 Energy Supply in Germany

As of 2010, Germany's primary energy supply of 14,057 petajoule (PJ) relied on five major sources, namely coal, mineral oil, natural gas, nuclear power and renewables (see Figure 2-1). The advantages of the processes using these resources, both of fossil and renewable nature, are the benchmark against which new processes for the supply of energy have to be measured. Three of the main conditions for a sustainable energy supply are economic viability, security of supply and environmental impact (EnWG 2005).

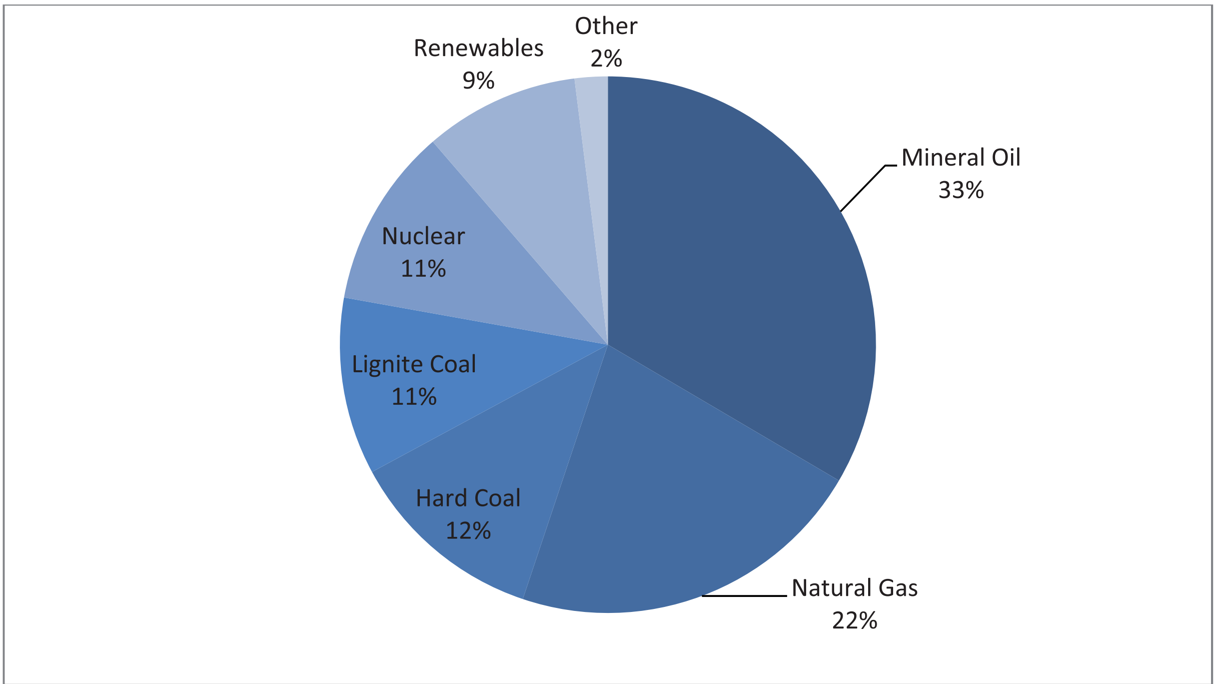

Figure 2-1: Primary energy supply in Germany in 2010 (AGEB 2011)

While economic viability refers to expected price and cost developments, domestic abundance or reliability of imported resources play a part in the maximization of supply security. An often-quoted measure in this field is the “reserves-to-production ratio”, which expresses how long economically extractable reserves are expected to last at current production rates and current prices. While this ratio is often quoted to predict the time-frame in which resources will be available for further energy generation, the resulting number of years has often grown, rather than shrunk, over time (Erdmann/Zweifel 2007, p. 126). This is due to the fact that economic extraction depends on the value of the produced resources, i.e. when resource prices rise, the amount of economically extractable resources grows. High prices also increase the incentive to search and discover new deposits of resources. In spite of these shortcomings, the reserves-to-production ratio usually gives an indication of the availability of energy resources.

In addition to such considerations, the prospects of resources in the energy mix have also come to increasingly depend on the perceived gravity of environmentally hazardous side-effects. As the importance of environmental considerations has had an increasing effect on decision-making in the energy business, the composition of the German energy mix has been undergoing a continuous change in the last 20 years (BMU 2011, p. 7). In order to give an overview of the current prospects of energy processes in Germany, the five most significant energy resources will be discussed with regard to their expected developments in terms of economic competitiveness, supply security and environmental impact.

2.1.1 Coal

Hard and lignite coal, Germany’s traditional domestic energy resources, supplied 22.8 % of primary energy supply in 2010. The exploitation of domestic surface mining pits has made Germany the greatest lignite coal producer in the world. The reserves-to-production ratio implies that a production at this level should be possible for at least another 200 years, with significantly more lignite available if the overall level of energy cost increased sufficiently to justify further exploitation (Erdmann/Zweifel 2007, p. 254). Due to economic transportation limitations, the production of electricity from lignite coal is restricted to areas close to the lignite surface mining pits (Wolk, et al. 2008a, p. 18). As reserves in the historically most significant area of exploitation, in central Germany, are nearing exhaustion, lignite coal production is increasingly focused on the more abundant fields in the Rhineland and the Lausitz (see Table 2-1).

In spite of the significant production and reserves, “cap-and-trade”[1] of CO_2 emissions is expected to significantly deteriorate lignite coals competitiveness if prices for CO_2 certificates were to rise.

[1] Cap-and-trade refers to a legal limitation of CO_2 emissions that results in the trading of CO_2 emission certificates (Erdmann/Zweifel, 2007, p. 353)

Table 2-1: German lignite coal production
(Pfaffenberger/Ströbele 2010, p. 97)

Million tons	1950	1960	1970	1980	1990	2000	2005	2008
Rhineland	64	81	93	118	102	92	97	96
Lausitz	36	84	134	162	168	55	59	58
Central Germany	101	142	127	96	81	16	19	19
Helmstedt	8	7	5	4	4	4	2	2
Hesse	3	4	4	3	1	0	0	0
Bavaria	2	4	5	5	0	0	0	0
Total German Production	213	322	369	388	357	168	178	175
Employees (in 1,000)	106	150	122	152	130	21	17	17

Where no lignite coal is immediately available, hard coal is used as it can be transported more efficiently due to its higher energy density. Domestic hard coal production, which used to take place in the Ruhr and Saar regions, has declined as depleting mines lead to rising production costs, rendering domestic hard coal increasingly scarce and expensive. To compensate for the declining amount of hard coal mined domestically, it is being imported to an increasing extent. Germany is considered part of the Atlantic coal market, which is being supplied from countries such as Columbia, South Africa, Russia, Poland, Venezuela and the United States of America (Pfaffenberger/Ströbele 2010, p. 100). While the reserves-to-production ratios of hard coal in these countries forecast that the current pace of extraction could be maintained for more than two hundred years, hard coal prices have shown an even greater fluctuation than those for mineral oil in recent years. In percentage terms, hard coal prices rose by 423.8 % from November 2005 to July 2008, as compared to 239.5 % for "Brent" crude oil (see Figure 2-2).

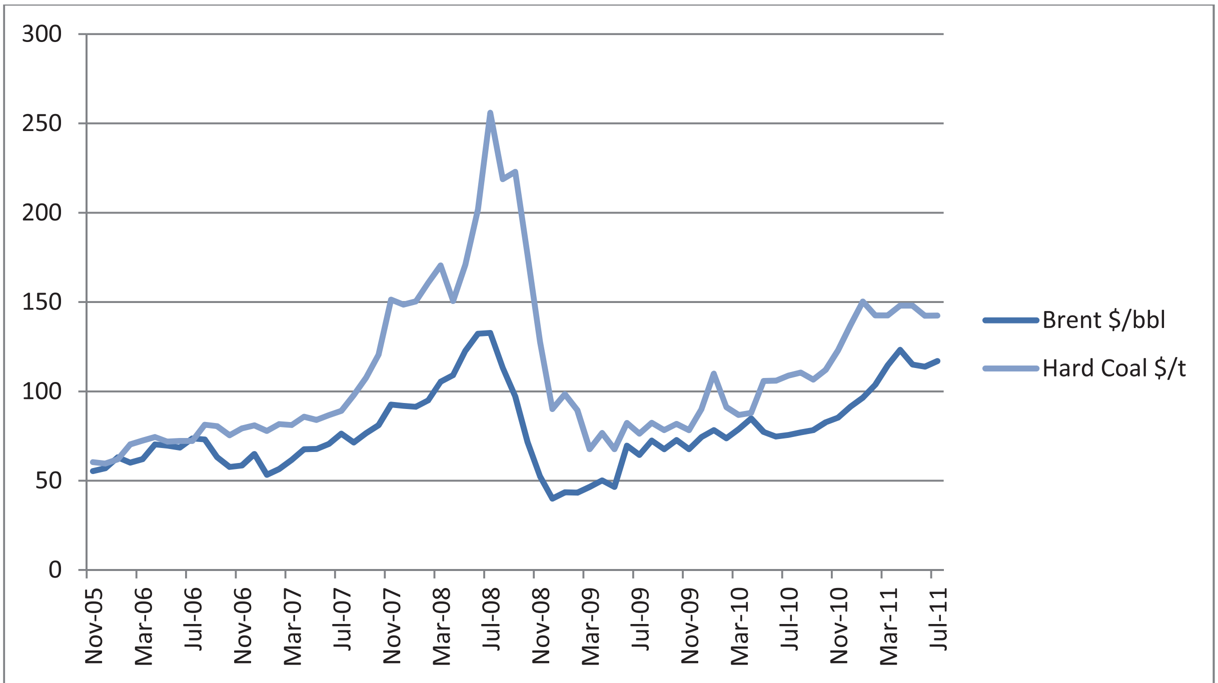

Figure 2-2: Development of hard coal and crude oil prices
(BGR 2005-2011)