A standardized methodology for the techno-economic evaluation of alternative fuels – A case study

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ABSTRACT

Greenhouse gas emissions in the transport sector can significantly be reduced by replacing fossil based fuels with green alternatives. Various alternative fuel concepts have been developed differing in used sustainable feedstock, synthesis technology and final fuel characteristics. Whether these fuels can succeed in the market will depend on the fuel net production costs, the expected cost reduction potentials and the political intention to mitigate climate change. Results of previous studies for the techno-economic assessment of alternative fuels are difficult to compare due to significant differences in the applied methodology, level of detail and key assumptions in terms of economic factors and market prices. In this work, a standardized methodology for techno-economic analysis of fuel production processes is presented and exemplarily applied on sustainable fuels from Fischer-Tropsch (FT) synthesis. The methodology was adapted from a best practice approach from chemical industry and consists of three main steps: A) literature survey on feasible production designs, B) flowsheet simulation and C) techno-economic assessment with the in-house software tool TEPET (Techno-Economic Process Evaluation Tool). It is shown that the standardized approach enables qualitative and quantitative statements regarding the technical and economic feasibility of fuel synthesis concepts including the identification of the appropriate fuel production concept due to predefined framework conditions. Results from the case study on green FT fuels reveal that Biomass-to-Liquid (BtL) concepts have lowest production costs at high electricity costs, whereas the Power-to-Liquid (PtL) and Power and Biomass-to-Liquid (PBtL) concepts are superior at low electricity prices. Fuel production costs in the range of 1.2 and 2.8 $€_{2014}$/l were estimated.

1. Introduction

In 2012, 95 % of the energy consumed in European transport was supplied by crude oil products [1]. Greenhouse gas (GHG) emissions from transportation account for about 25 % of total European GHG emissions [2]. In order to keep global warming below 2 °C, the European Union has set binding targets for cutting GHG intensity of fuels by 6 % compared to 2010 [3] and to increase the share of renewable energies in the transport sector to 10 % until 2020 [4] with special requirements regarding indirect land use change [5]. While electric vehicles may become a viable option to reach these goals in private car traffic, aviation and heavy duty transportation will continue to rely on liquid fuels due to the required high volumetric energy density and the high investment costs for changing today's engine technology and infrastructure [6]. It is therefore expected that a large amount of alternative "drop-in" fuels are required to significantly decrease the carbon footprint in these transportation sectors. Most alternative fuels available on the market today are so-called 1st generation fuels, which predominantly are made from energy crops raising the issue of competition for farmland and low technical expansion potential in Europe. Hence, future fuels have to preferably be made from renewable electricity, residues and waste wood to decrease the effect of indirect land use change.

Multiple 2nd generation production paths for alternative liquid fuels have been developed in the recent years such as Fischer-Tropsch fuels, Dimethylether (DME) based fuels such as Methanol-to-Gasoline (MtG) or alcohols (ethanol, butanol), to mention only a few examples. Though, the "optimal" alternative future fuel remains to be identified. One the one hand, requirements regarding main fuel characteristics and total fuel demand varies considerably among the specific application areas (road transport, aviation, astronautics etc.). On the other hand, political framework conditions such as support schemes and tax advantages significantly affect the development of the fuel market and therewith also predefine the feasibility of alternative fuels. In order to evaluate and compare the prospects of emerging alternative fuel concepts, the German Aerospace Center (DLR) has launched the strategic project "Future Fuels". One main focus is on economic performance parameters such as capital investment cost and fuel production costs, which are considered to be one of the major factors for the market success of alternative fuels.

A large number of techno-economic studies on a wide range of different alternative and synthetic fuels already exist, which typically apply a methodology adapted from the power or chemical industry. Worth mentioning are the fundamental works on process economics of Peters et al. [7], Ulrich et al. [8], Smith et al. [9] and Turton et al. [10]. Despite the similar economic approach applied in cost calculation studies on alternative fuels, a common concern is the comparability of results. This issue was addressed by Haarlemmer et al. [11] using the example of biofuels production via Fischer-Tropsch synthesis from biomass (Biomass-to-Liquid, BtL), coal (Coal-to-Liquid, CtL) and gas (Gas-to-Liquid, GtL). The authors showed by comparing more than 20 recently published techno-economic studies that a reasonable comparison is impossible not only due to different methodologies used, but also because of unequal source data (cost data, ratio factors and economic assumptions such as plant lifetime, interest rate and inflation). Another problem is the lack of calculation details in most studies making it difficult to understand the underlying assumptions of the cost calculation [12]. Hence, economic results can hardly be normalized in terms of e. g. plant scale, depreciation method and economic assumptions such as raw material market prices and equipment costs.

A more consistent approach is to compare various synthetic fuel production option by applying a kind of superstructure-based methodology as proposed in the studies by Cheali [13] and Maravelias et al. [14] [15]. The drawback of superstructure studies is that process steps typically are very simplified in order to obtain a mathematical correlation which can be used in commercial or new developed mathematical optimization algorithms. Great simplifications bear the risk that process limitations due to thermodynamic phenomena such as catalyst coking or the effect of recycle streams on reaction kinetics are neglected or underestimated.

Since no standardized methodology for comparing alternative fuels exists at present, a reliable and unbiased comparison schema for alternative fuels was developed in the course of the Future Fuel project. This paper presents first results in terms of a transparent methodology for the estimation of fuel net production costs (NPC), which was implemented in the in-house tool TEPET (Techno-Economic Process Evaluation Tool). The methodology is characterized by a high of level detail including experimental investigations of key process steps. Starting from a detailed description of the methodology for the techno-economic evaluation in chapter 2, the TEPET tool is applied in a case study on a comparison of key economic measures of three different Fischer-Tropsch fuel synthesis routes based on various feedstocks (Chapter 3). The case study includes a detailed literature survey on possible process pathways, descriptions of the implemented process models and basic information about the applied heat integration. Finally, a comparison of results with previous techno-economic studies of Fischer-Tropsch fuels is made and a brief discussion of uncertainties regarding the applied methodology is given.

2. Methodology of techno-economic evaluation

Figure 1 shows a block diagram providing a rough overview of the developed methodology for the standardized techno-economic evaluation of alternative fuels.

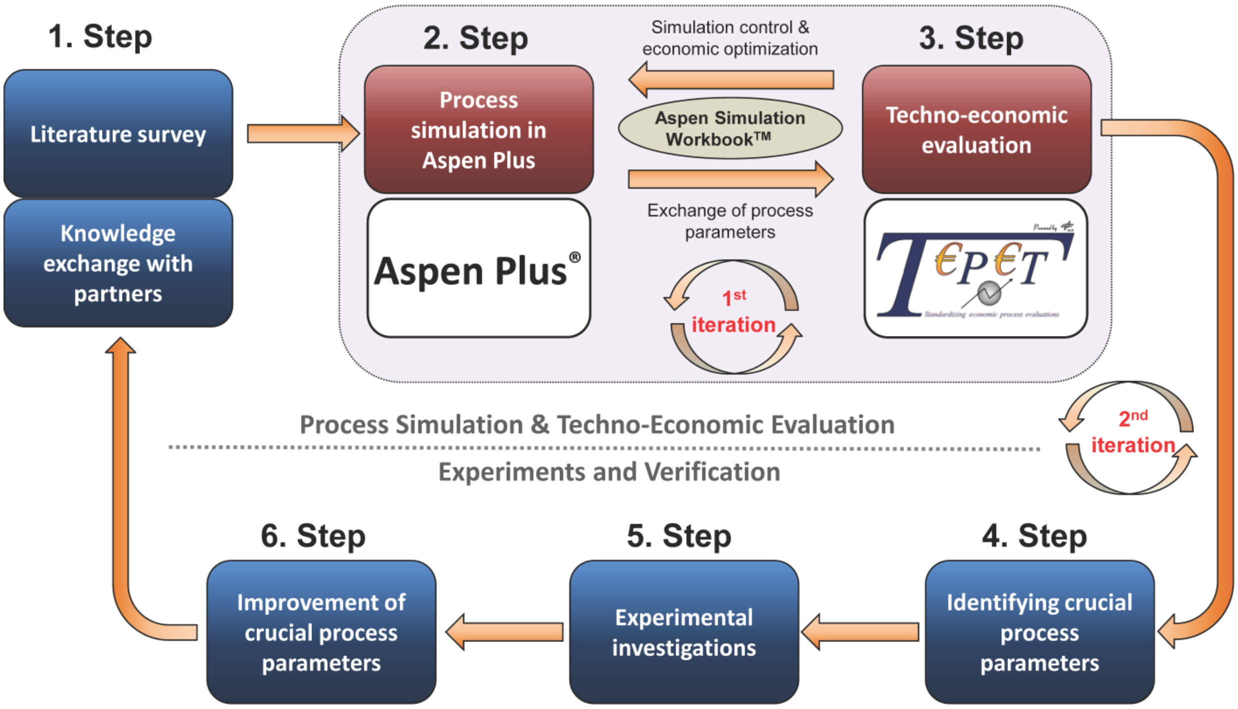

Figure 1: DLR methodology for Techno-Economic Evaluation

The DLR approach consists of six major steps, whereby the first three are discussed in this work. Initially, an extensive literature survey on the fuel production path to be investigated is carried out. The focus is on available technologies and process concepts as well as on economic data for key process equipment. In addition, technical and economic data from associated research and industrial partners is used. As a second step, a detailed process simulation is implemented for the most promising fuel production routes using commercial Aspen Plus® software. Implemented process simulations are characterized by a high level of detail enabling a reasonable investigation of the interaction of crucial production steps in terms of operation conditions (temperature, pressure etc.), energetic efficiency and optimal process design. The process simulations are heat integrated to minimize utility costs by designing an optimized heat exchanger network based on results from pinch-point analysis. In the third step, the thermally optimized simulations are directly connected to TEPET by using the Aspen add-on Aspen Simulation Workbook™. Because of this interlinking, NPC calculation is automatically updated when process simulation parameters and settings are changed. Furthermore, sensitivity analyses of key process parameters can be easily conducted by controlling the process simulation with TEPET. The methodology used for cost calculations was adapted from a best-practice approach from the chemical industry [7] [9] [16], since fuel production on a large scale can be considered to be very similar to common petro-chemical processes. Though, the methodology was improved and extended by the authors in terms of additional economic measures such as experience curve effects. Key economic parameters calculated are total and equipment specific capital expenditures (CAPEX), operational expenditures (OPEX) as well as fuel net production costs (NPC). Additionally, the effect of economy of scale is examined and the most sensible input parameters are identified. The findings of the techno-economic evaluation are used to modify the simulation process design in order to minimize NPC, which can be seen as a first iteration loop within the procedure. Subsequent, crucial process steps having a large impact on NPC are identified (step 4) and in the following investigated (step 5) in terms of small-scale experiments in order to verify technical feasibility of chosen operation conditions. If model assumptions cannot be verified by experimental work, the process design or process parameters are modified resulting in a second iteration loop. The present work deals exclusively with the first three steps with focus on the first iteration loop (step 2 & 3). Steps four to six will be discussed in a subsequent study.

2.1 Process simulation

The main purpose of setting up process simulations is the in-depth investigation of interdependences of key production steps within the fuel production route with regard to process parameters (T, p, etc.) and economic cost saving potentials. Process models of this work employ all equipment required to reproduce changes of chemical composition and thermodynamic state of the main process streams. This includes all reactors, burners, heat exchangers, pumps and compressors, flashes and valves. Other auxiliary equipment characterized by no significant potential for heat and material integration are simply modeled as black box with specific electricity and heat demands. Though, electricity generation as well as steam production from waste heat and off gases is modeled as well. Process models are heat integrated by applying the pinch analysis method [17] [18] and appropriate heat exchanger networks are designed in order to minimize external heating and cooling demand.

2.2 Cost estimation methodology

A simplified summary of the cost estimation methodology used in TEPET for estimating NPC is illustrated in

Figure 2.

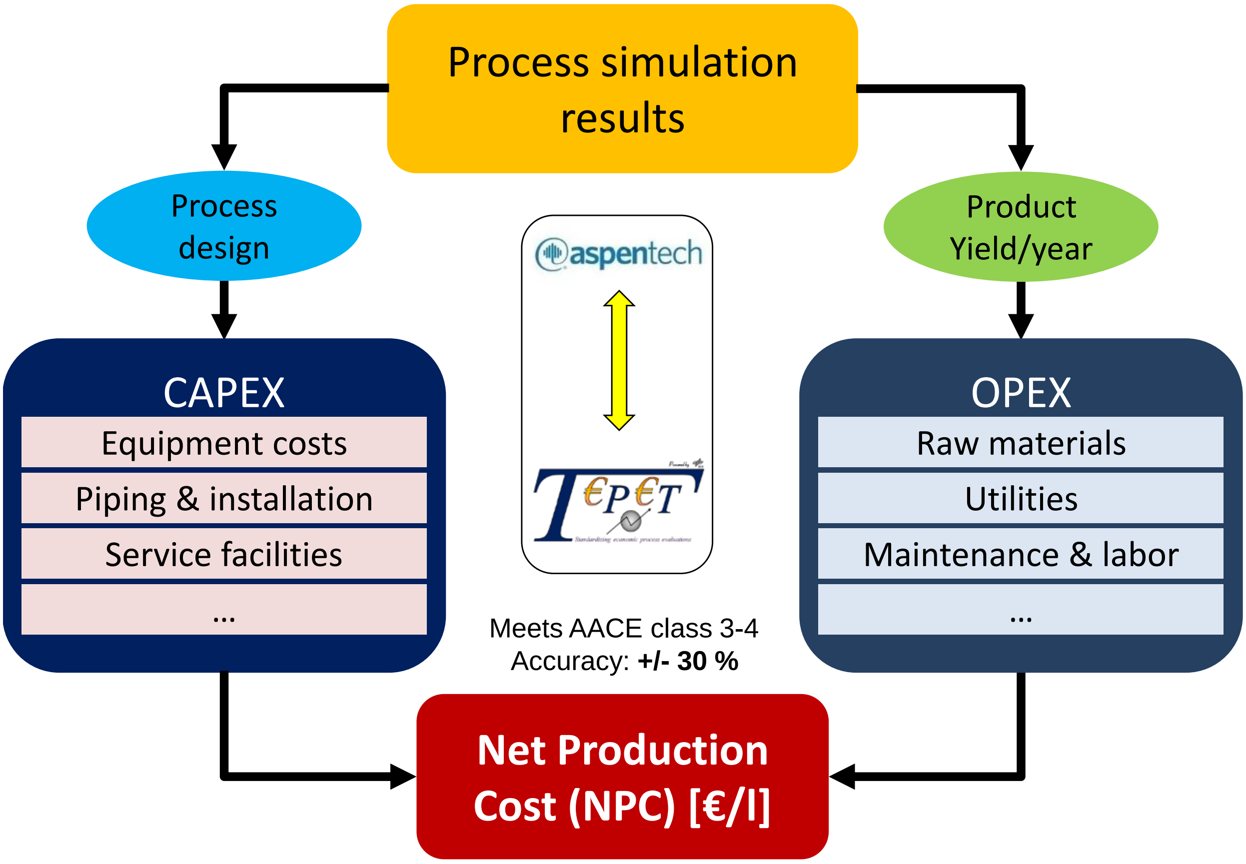

Figure 2: Simplified scheme of cost estimation methodology in TEPET

The methodology for estimating CAPEX, OPEX and NPC is presented in the following subsections. The accuracy of cost estimation is expected to be +/- 30 % according to class three and four of the classification system of AACE (Association for the Advancement of Cost Engineering) [19].

Capital investment costs (CAPEX)

Fixed capital investment (FCI) costs consist of equipment costs (EC) and further capital requirements in the construction phase. EC for all installed units are calculated in TEPET according to Equation (1), which was reproduced from Peters et al. [7] and further developed by the authors taking into account experience curve effects based on the work of the National Energy Technology Laboratory [20] and Smith et al. [21].

$$EC_i = f_i(S_{i,1}; S_{i,2}; \dots; S_{i,k}) * \left(\frac{CEPCI}{CEPCI_{ref}}\right) * F_{pre,i} * F_{mat,i} * \left(1 - L_i^{log_2(n)}\right) \quad , \quad i, k \in \mathbb{N} \qquad (1)$$

$$f_i(S_{i,1}; S_{i,2}; \dots; S_{i,k})_{example,(k=1)} = f_i(S_i) = EC_{ref,i} * \left(\frac{S_i}{S_{ref,i}}\right)^{d_i} \qquad (2)$$

f_i describes an equipment specific cost function which assigns equipment costs to every item i in the process simulation. Depending on the type of equipment and the source of the reference data, several input variables $S_{i,k}$ (volume, throughput, temperature, etc.) are taken into account. The required capacity is distributed over a number of parallel units with same size, if the single unit capacity is restricted. An example of cost function for estimating equipment costs frequently used in scientific literature with only one input variable (k=1) is given in Equation (2).

$EC_{ref,i}$ and $S_{ref,i}$ describe equipment costs and a characteristic capacity, respectively, of a reference unit i, whereas S_i is the actual equipment size extracted from the process simulation via Aspen Simulation Workbook^{TM}. Economy of scale is considered by the equipment specific scale factor d_i. A database consisting of cost functions for main chemical process equipment as well as for fuel synthesis equipment was implemented and included in TEPET based on available data from scientific reference literature (see *Table 5*). In order to account for inflation and temporal cost variations of equipment, the Chemical Engineering Plant Cost Index (CEPCI) is used to update old data with respect to the chosen reference year. Since the CEPCI is published on an U.S. dollar basis, reference equipment costs given in Euro (€) are first converted to US$ using the specific exchange rate of the reference year before the CEPCI is applied. Additional expenses on equipment due to high operation pressure or material requirements are considered by the additional multipliers $\mathrm{F_{pre}}$ and $\mathrm{F_{mat}}$, respectively. Optionally, learning and experience curve effects can be accounted for by considering the term $\left(1 - L_i^{log_2(n)}\right)$ (see Equation (1)) based on an equipment specific experience rate L and the total number of manufactured equipment units n. Experience curve effects have to be handled carefully, since it is difficult to forecast the development of equipment costs of novel technologies. An example techno-economic evaluation on biodiesel reformers including experience curve effects is given in [23]. Fixed capital costs (FCI) were calculated according to Equation (3) by multiplying equipment costs by pre-defined ratio factors $\mathrm{F_{eco,i,j}}$, which are summarized in *Table 1* along with typical values for fluid processing plants in the chemical industry [7].

$$FCI = \sum_{i=1}^{m} EC_i * \left(1 + \sum_{j=1}^{10} F_{eco,i,j}\right) * \left(1 + \sum_{j=11}^{12} F_{eco,i,j}\right) \quad , \quad TCI = \frac{FCI}{0.9} \tag{3}$$

Some of the ratio factors may be neglected, if they are not relevant for the scope of the techno-economic evaluation or if they are already included in the given reference equipment costs (e.g. installation costs).

Table 1: Ratio factor for estimating FCI of fluid processing chemical plants reproduced from [7]

Indirect cost items $F_{ind,i,j}$	*j*	*Basis*	*Typical Value*
Equipment installation	1	EC	0.47
Instrumentation and control	2	EC	0.36
Piping (installed)	3	EC	0.68
Electrical (installed)	4	EC	0.11
Buildings including services	5	EC	0.18
Yard improvements	6	EC	0.1
Service facilities (installed)	7	EC	0.55
Total direct plant costs (D)			
Engineering and supervision	8	EC	0.33
Construction expenses	9	EC	0.41
Legal expenses	10	EC	0.04
Total direct and indirect costs (D + I)			
Contractor's fee	11	D + I	0.05
Contingency	12	D + I	0.1

Total capital investment (TCI) is estimated by predicting that 10 % of TCI is required as working capital.

In order to calculate equivalent annual capital costs (ACC), both the FCI and the required working capital have to be considered (Equation (4)). The first term in the brackets arises from applying the annuity method on the FCI assuming that the value of the plant is zero at the end of plant life. Since working capital does not depreciate in value, only the interest rate (IR) has to be paid on the working capital resulting in the second term in Equation (4).

$$ACC = FCI * \left(\frac{IR * (1 + IR)^y}{(1 + IR)^y - 1} + \frac{IR * y}{9} \right) \tag{4}$$

Operational expenditures (OPEX)

Operational expenditures can be broken down in costs for raw materials and utilities (referred to as "direct OPEX") and other operational costs including for example maintenance, labor, insurances and taxes (referred to as "indirect OPEX"). Direct OPEX are calculated based on results from the process simulations and average annual market prices in the base year as shown in Equation (5). If only older market prices are available, a commodity price index (CPI) is used to update price data. Commonly used commodity price indices are the *Rogers International Commodity Index*® [24] and the World Bank Commodity Price Data (The Pink Sheet) [25]. Both indices are further divided into sub-indices, which reflect different commodity segments allowing a more accurate update of market prices. Revenues from selling by-products, heat and electricity are accounted for in the same way.

$$\begin{aligned} \sum OPEX_{dir} \left(\frac{€/\$}{year} \right) = {} & \textstyle\sum_{i=1}^{m} \dot{m}_{R\&B\_i} * c_{R\&B\_i} * \left(\frac{CPI_i}{CPI_{ref,i}} \right) + \sum_{j=1}^{n} E_{power_j} * c_{power_j} + \\ & \textstyle\sum_{k=1}^{p} W_{heat_k} * c_{heat_k} \end{aligned} \tag{5}$$

Since power and heat streams crossing the system boundaries can be subject to different market prices (e.g. stock market price versus granted feed-in remuneration for electricity according to the German Renewable Energy Act [26]), each energy stream is accounted for separately. It shall be noted that market prices $c_{RM\_BP\_i}$, c_{power_j} and c_{heat_k} for exported raw materials, by-products, power and heat, respectively, have by definition a negative sign.

Indirect OPEX include all additional expenses originating from plant operation such as maintenance, labor and administration. Since exact costs are difficult to predict, typical estimates are used based on historical data form the chemical process industry [7], which are summarized in *Table 2*. It shall be noted that indirect OPEX is by definition directly linked to CAPEX. Annual costs for operating labor (OL) are calculated based on average specific labor costs (c_{labor}) in the German industry [27]. Man-hours (h_{labor}) are predicted as a function of plant capacity and the number of principle processing steps according to the work of Peters et al. [7] (functions used are given in the supplementary information chapter B).

Table 2: Ratio factors for estimating indirect OPEX of fluid processing chemical plants reproduced from [7]

Investment item	***j***	***Basis***	***Typical Value***
Operating supervision	1	OL	0.15
Maintenance labor	2	FCI	0.01-0.03
Maintenance material	3	FCI	0.01-0.03
Operating supplies	4	M[a]	0.15
Laboratory charges	5	OL	0.2
Insurance and taxes	6	FCI	0.02
Plant overhead costs [PO]	7	TLC[b]	0.6
Administrative costs	8	PO	0.25
Distribution and selling costs	9	NPC	0.06
Research and development costs	10	NPC	0.04

[a] M = Maintenance labor & maintenance material

[b] TLC = total labor costs consisting of operating labor, operating supervision and maintenance labor

Net production costs (NPC)

The net production costs (NPC) were calculated according to Equation (6).

$$NPC\left(\frac{€}{l}\right) = \frac{ACC + \sum OPEX_{ind} + \sum OPEX_{dir} + h_{labor} * c_{labor}}{\dot{m}_{fuel} * \rho_{fuel}{}^{-1} * \frac{\omega_{fuel}}{\omega_{reference}}} \qquad (6)$$

The indirect OPEX are calculated based on data from *Table 2*. All levelized cost flows are normalized with the annual fuel output $\dot{m}_{fuel}$ and fuel density ρ_{fuel}. In order to compare calculated NPC with fossil reference fuels, the ratio of the energy density (ω in Equation (6)) is considered.

3. Case study – Techno-economic evaluation of sustainable Fischer-Tropsch fuels

The methodology presented in chapter 2 was applied on fuel production concepts based on Fischer-Tropsch (FT) synthesis, one option to produce alternative fuels from a large variety of feedstocks. Fischer-Tropsch fuel production is a state-of-the-art process, which has been applied since 1925 [28], though, initially with coal as feedstock. A large number of studies are available on the techno-economic assessment of different sustainable FT routes using biomass as feedstock (Biomass-to-Liquid - BtL), hydrogen and carbon dioxide as feedstock (Power-to-Liquid - PtL) and a combination of the PtL and BtL concept (Power and Biomass-to-Liquid – PBtL). Various BtL concept designs with focus on different gasification technologies based on low-temperature, cobalt-catalyzed FT-synthesis have been analyzed in a superstructure approach by the groups of Tijmensen/Hamelinck/Faaij/van Vliet et al. (Utrecht University) [29] [30] [31] and Haarlemmer/Peduzzi/Seiler et al. (CEA) [12] [11]. In the same manner, Hannula and Kurkela et al. (VTT) investigated different process designs of fluidized bed biomass gasifiers in combination with liquid transportation fuels by FT-synthesis and methanol-to-gasoline (MtG) [32] [33]. Kerdoncuff/Trippe et al. (KIT) published studies on the technical and economic performance of the so-called bioliq® BtL process, in which biomass is pre-processed in decentralized pyrolysis units and liquid fuels are produced in a large centralized plant by entrained flow-gasification and the FT or MtG synthesis [34] [35]. Worth mentioning are also the works of the groups of Swanson/Becker/Braun et al. (NREL) [36] [37] [38] and Larson/Kreutz/Baliban/Floudas et al. (Princeton University) [39] [40] [41], who published comprehensive economic studies on BtL and CtL concepts with simultaneous electricity production and district heat supply.

On the contrary, only a few studies exist on the performance of PtL and PBtL concepts. Becker et al. designed a PtL FT-process, where the syngas for cobalt-catalyzed low temperature Fischer-Tropsch (LTFT) synthesis is supplied by high-temperature co-electrolysis of CO_2 and H_2O in a solid oxide electrolyzer cell (SOEC) [38]. A similar approach was chosen by König et al, though, proton exchange membrane (PEM) electrolysis is applied for H2 production and CO2 is activated and converted to CO in a high-temperature reversible water-gas shift reactor [42] [22]. PBtL concepts typically stem from basic BtL concepts, where hydrogen is added prior to the FT-synthesis in order to make redundant the water-gas shift reaction (e. g. Seiler et al. [43]) or a reverse water-gas shift reactor is used to realize a very high carbon conversion by activating CO_2, as published by Baliban et al. [41].

Net production costs (NPC) of the mentioned studies vary in a wide range between 0.57 and 4.7 €/l_{GE} (liter gasoline equivalent) depending on the applied methodology, assumed raw material and equipment costs, scale of plant, learning curve effects and other factors. To the author's knowledge, no detailed scientific study exists so far on a comparison of BtL, PtL and PBtL FT-concepts among each other in terms of strengths and weaknesses as well as key economic parameters. In this work, the focus is both on the technical and energetic performance (efficiencies, carbon conversion etc.) and on CAPEX, OPEX and NPC. Furthermore, effects of economy of scale on NPC were investigated and an extensive sensitivity analysis was carried out with TEPET in order to identify the most significant cost-drivers of the three concepts.

3.1 Concept description and literature survey

Figure 3 shows the system boundaries and a simplified block flow diagram of three concepts marked as PtL, BtL and PBtL. A distinction is made between chosen process options (blue color), interesting alternative process options not considered (ochre color) and required process options outside the system boundary (grey color). In order to decrease complexity of the illustration, the block flow diagram is divided into a syngas supply and fuel synthesis system.

Regarding syngas supply, a carbon and a hydrogen source is required for liquid fuel production. In the BtL concept, syngas is supplied solely by thermochemical conversion of biomass. Depending on the nature and humidity of the biomass feedstock as well as the selected gasification technology, several pre-treatment steps such as drying, grinding, pyrolysis or torrefaction are required [44]. The two last mentioned processes aim to remove residual moisture from the biomass, to increase the energy density and to ensure a better feedstock handling by producing a pumpable slurry (pyrolysis) or increasing grindability (terrefaction). Currently, fixed-bed, fluidized bed and entrained flow gasifier are mainly used for biomass gasification, though, only the two last mentioned offer the potential for scaled up in the 50 – 1,000 MW_{th} range [45] [46] [47] [48].

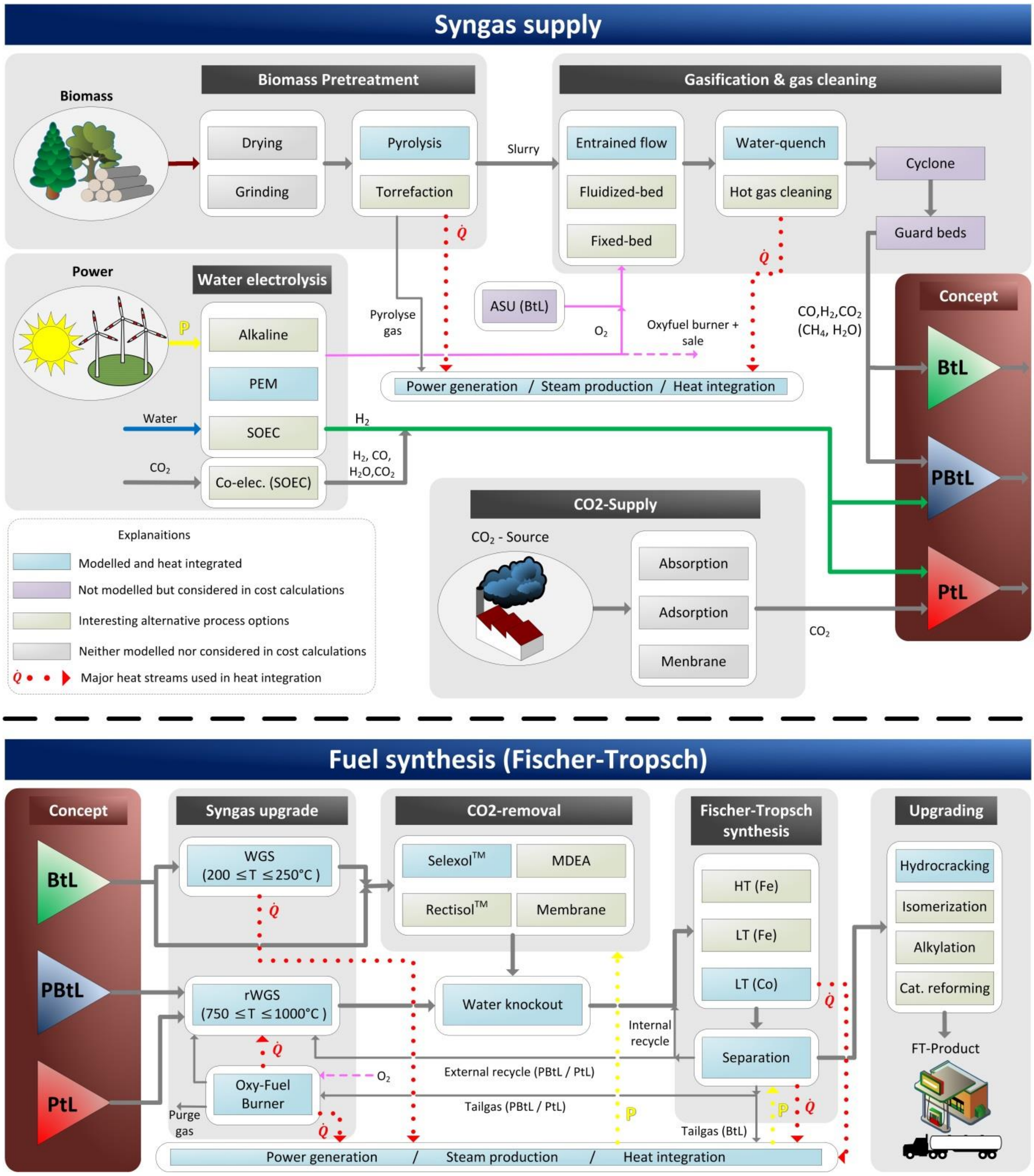

Figure 3: Block flow diagram and system boundary of BtL, PtL and PBtL concepts

In this study, entrained flow gasification was selected due to the better scale-up potential, the higher technology readiness level and the lower methane and tar concentration in the raw gas due to the high operation temperature of above 1100 °C. Entrained flow gasification requires an elaborate biomass pre-treatment, since a pumpable feedstock is required for the feed-in at elevated pressures (> 20 bar). Hence, fast pyrolysis was selected as appropriate pre-treatment process in which biomass is mixed with hot sand at a temperature of around 550 °C [35] [49] [50]. The solid and liquid product fraction is mixed to the so-called slurry and utilized in the gasifier by partial oxidation of the feed using either air or oxygen as oxidizer. Raw gas from gasification is rapidly cooled down by water quenching, whereby most particles and impurities including most water-soluble pollutants such as hydrogen chloride and ammonia are already removed [12]. Remaining char, dust particles and impurities such as H_2S are separated and removed from the wet syngas in an arrangement of cyclones, guard beds and filters. Another prospective technology to reduce exergetic losses may be hot gas cleaning by for example high-temperature gas filtration using ceramic filter media [51]. However, hot gas cleaning is not a proven technology and not commercially available [30] and additional research efforts are required to achieve a high cleaning effectiveness.

The cleaned raw gas is in general characterized by a shortage of hydrogen. Hence, a downstream exothermic water-gas-shift (WGS) reactor is required adjusting the H_2/CO ratio before FT synthesis. The reaction mechanism is given in Equation (7) [52]. Typical operation temperature levels are in the range between 190 and 250 °C [28].

$$CO + H_2O \leftrightarrow CO_2 + H_2 \quad , \quad \Delta H_R^0 = -41.2\ kJ/mol \tag{7}$$

As a last step of syngas upgrade in the BtL concept, carbon dioxide has to be removed prior to the FT-synthesis to avoid accumulation of CO_2 in the system. State-of-the-art technologies for CO_2 removal are chemical absorption using amines (MEA/MDEA) as solvent, physical absorption using for example Rectisol® or dimethyl ethers of polyethylene glycol (e.g. Selexol^{TM}) as solvent or membrane gas separation [53] [54]. Physical absorption is superior to chemical absorption in the case of high partial pressures of CO_2 due to lower energy requirements for solvent regeneration. Selexol^{TM} is recommended as the most energy and cost efficient physical solvent [55] [56] [57] and is therefore considered as appropriate CO_2 removal technology in the case study.

Syngas in the PtL route is composed of hydrogen from water electrolysis and CO_2 originating either from industrial processes or air. The appropriate separation process depends on the CO_2 concentration in the feed stream. Adsorption, absorption or membrane technologies may be the most economic feasible option. CO_2 supply is not further discussed in this work, but will be a major topic in subsequent studies. Common electrolysis technologies are alkaline electrolysis, PEM electrolysis and high-temperature electrolysis with SOEC. The TRL level decreases significantly in that order [58]. This work focuses on PEM electrolysis, because of the superior dynamic operation behavior offering the potential to connect the device directly to fluctuating power sources. Carbon dioxide has to be activated and converted to CO by the reverse water-gas-shift (rWGS) reaction at elevated operation temperature (>750°C) ensuring an appropriate CO yield [52]. The rWGS reaction itself follows the reverse mechanism as shown in Equation (7). An interesting prospective for syngas production is SOEC co-electrolysis as proposed by Becker et al. [38] making redundant the rWGS reaction. Though, SOEC co-electrolysis is still at an early development stage and additional research is required in order to reach market maturity.

The syngas supply in the PBtL concept is a combination of the BtL and PtL route. Raw gas from biomass gasification is enriched with hydrogen before the rWGS reactor. No external carbon dioxide and oxygen source is needed. *Table 3* summarizes the main characteristics of the investigated concepts.

Table 3: Main characteristics of the three investigated concepts

Concept	***Carbon source***	***Hydrogen Source***	***Syngas supply***	***Syngas upgrade***	***Carbon recycling***
Power-to-Liquid (PtL)	CO_2	H_2O	CO_2 separation and electrolysis	rWGS	Yes
Biomass & Power-to-Liquid (PBtL)	Biomass	H_2O	gasification and electrolysis	rWGS	Yes
Biomass-to-Liquid (BtL)	Biomass	Biomass/(H_2O)	gasification	WGS	No

The fuel production section is the same for all concepts and comprises a Fischer-Tropsch (FT) reactor and a product separation and upgrading section. A reaction mechanism of the underlying polymerization reaction in FT-synthesis is given in Equation (13) [41].

$$n \cdot CO + 2n \cdot H_2 \rightarrow (-CH_2-)_n + n \cdot H_2O \quad , \qquad n \epsilon \mathbb{N} \qquad , \quad \Delta H_R^0 = -n * 152 \ kJ/mol \qquad (8)$$

According to Equation (8), FT-synthesis requires a H_2/CO ratio of above 2 in the feed stream. The FT-product, so-called syncrude, consists of a large variety of different species such as alkanes, alkenes, alcohols, carbonyls and carboxylic acids. A good estimate of the syncrude carbon number distribution is given by the Anderson-Schulz-Flory (ASF) distribution as shown in Equation (9) [28].

$$x_n = (1 - \alpha) \cdot \alpha^{(n-1)} \tag{9}$$

The molar fraction x_n of each product with carbon number n is related to the chain growth probability α, which is a statistical measure predicting whether chain propagation or termination occurs. The chain growth probability α depends on the reactor design, the operation conditions and the used catalyst. A distinction is made between low temperature FT-synthesis (LTFT) with iron or cobalt based catalysts and high temperature FT-synthesis (HTFT) based on primarily iron catalysts with typical temperature conditions of 200 - 240 °C and 300 - 350 °C, respectively [28] [59] [60] [61]. HTFT is typically applied for gas, olefins and gasoline production, whereas product distribution of LTFT has its maximum in the kerosene, diesel or wax fraction. Three main reactor designs namely fixed bed, fluidized bed (circulating and stationary) and slurry reactor are available. Strengths and weaknesses of FT designs are elaborately discussed in the work of de Klerk [28]. Since it was aimed to maximize the liquid fuel output, LTFT in a fixed bed reactor using a cobalt based catalysts was investigated in this work. In order to comply with common fuel standards, further fuel treatments such as hydrocracking, catalytic reforming, isomerization and alkylation are applied [28] [62] [63]. Beside product separation, only hydrocracking is investigated in this work to convert the wax fraction into products with lower carbon number.

A light and a heavy gas fraction are obtained from product separation, which is referred to as recycle and tail gas, respectively (see *Figure 8* in SI). The recycle contains most of the unreacted educts, CO_2 and methane, and is reused in the FT-synthesis (internal recycle) and rWGS (external recycle), respectively [42, 28]. Thus, a higher carbon conversion along with a larger fuel output can be realized. Since temperature of WGS is not sufficient high to reactivate methane and CO_2, the BtL concept does not have an external recycle. Tail gas is burned to cover the heat demand of the rWGS (PBtL and PtL) or to produce electricity (BtL). As oxygen is available for free from electrolysis, oxy-fuel technology is used in the PBtL and PtL concept. Off-gas from the oxy-fuel burner is recycled into the rWGS reactor, which further increases total carbon conversion.

3.2 Process simulation model

Flowsheet models of each concept were implemented in Aspen Plus® software based on the Peng-Robinson equation of state with Boston-Mathias alpha function [24] [25], which is recommended for hydrocarbon processing applications such as gas processing, refining and petrochemical processes [64]. The plant capacities were initially estimated based on a predicted available specific biomass potential for Germany. A biomass feed-in of 98.3 MW_{th} was assumed for one BtL and PBtL plant (derivation can be found in chapter C of the supplementary information). Two PtL models (so-called small/large) were scaled such that a comparable fuel output was achieved corresponding to the BtL and PBtL model, respectively. It was predicted that each X-to-liquid plant is three weeks offline per year due to maintenance work resulting in a full load capacity factor of $cf_{plant} \approx 0.943$ or 8260 annual full load hours. Heat losses in piping and most equipment were neglected. Pressure drops in every section were roughly accounted for and modeled with an arrangement of valves and compressors. Subsequent, the modelling approach and assumptions for main process steps are discussed in detail. Simplified process flowsheets of the implemented models containing information on temperatures, pressures and mass flows are supplied in the supplementary information chapter D.

PEM electrolysis

The PEM electrolysis unit was simply modeled by a splitter with a conversion factor (with regard to water) of 67 % and operation conditions of 25 bar and 60 °C, respectively [65]. An energy demand of 4.3 kWh/Nm^3 (H_2) was used for electrolysis corresponding to an electrical efficiency (Power to LHV_{H2}) of approximately 70 % [58]. It was assumed that pure oxygen can be separated from the anode, which is than available for the use of oxy-fuel technology.

Pyrolysis and gasification section

Biomass was modeled as non-conventional compound with the molecular formula $C_6H_9O_4$ corresponding to lignocellulose in accordance with the work of Dahmen et al. [66]. Requisite pre-drying and grinding of biomass was neither modeled nor considered in the economic calculations. Fast pyrolysis was modeled based on a given yield distribution (yield reactor in Aspen Plus) for reaction conditions of 1 bar and 500 °C. Biomass is assumed to decompose according to the mechanism shown in Equation (10) (adapted from [66]).

$$\underbrace{C_6H_9O_4 \ + \ 0.69\,H_2O \ + 7g\,Ash}_{wet\ biomass} \quad \rightarrow \quad \underbrace{C_5H_{5.4}O_{1.1} + 7g\,Ash + 2.11\,H_2O}_{Slurry}$$
$$+ \ \underbrace{0.35\,CO \ + \ \ 0.07\,H_2 + 0.53\,CO_2 + 0.12\,CH_4 + 0.07\ \ H_2O}_{Pyrolysis\ gas} \qquad (10)$$

The slurry is separated from the pyrolysis gas in a flash arrangement. Heat for the endothermic pyrolysis reaction is supplied by a burner running on a mixture of pyrolysis gas and air (BtL) or oxygen (PBtL), which is modeled as a conversion reactor with known stoichiometry operating at 550 °C. The gasification part was modeled with a series of reactors. Because of the high operating temperature in the reactor, it is assumed that the produced syngas is in chemical equilibrium and that no tar is formed [67]. The nonconventional slurry component is converted into conventional gases in a yield reactor. Final syngas composition is calculated in a Gibbs reactor assuming total equilibrium at a pressure and temperature level of 30 bar and 1,200 °C, respectively. Heat demand for the endothermic reaction is covered by partial oxidation with pure oxygen. Syngas leaving the reaction chamber is quenched with water at 15 °C, resulting in a syngas temperature of 180 °C. The subsequent gas cleaning devices consisting of a cyclone (particle separation) and a number of guard beds (including ZnO beds for removal of Sulphur compounds) were not modelled but considered in the economic calculations.

WGS and rWGS reactor

Both WGS and rWGS reactor were modeled using a Gibbs reactor, as thermodynamic equilibrium is assumed [28] [68] [52]. WGS operation temperature was set to 230 °C to use the same water cooling cycle as for the FT-synthesis based on a water jacket operating at 25 bar (evaporation temperature ≈ 224

°C). rWGS temperature was fixed to 900 °C due to the favorable conversion rate of CO_2 at this temperature level [52]. Heat demand is covered by an oxy-fuel burner running on tail gases from product separation. Oxygen is delivered by the PEM electrolysis. The CO_2 rich off-gas from the oxy-fuel process is recycled in the rWGS reactor. Additional steam is added before the WGS reactor to avoid catalyst coking [69]. The amount of steam injected prior the WGS and rWGS reactor was estimated based on the thermodynamic carbon formation limits presented by Rostrup-Nielsen et al. [70] as a function of the H/C and O/C ratios in the feed. Since hydrogen is not available in the BtL concept, a small share of the hydrogen rich gas from the WGS reactor is send to a Pressure Swing Adsorption (PSA) unit in order to provide hydrogen for the hydrocracker. CO_2 is removed by a Selexol^{TM} unit assuming a separation efficiency of 90 % [71] [53]. A component separator simulates the Selexol unit. Power requirements were estimated using a specific electricity demand of 74 $kJ/kg_{CO2,removed}$ [30].

FT reactor

A stoichiometric reactor simulates the Fischer-Tropsch synthesis. Only alkanes were considered as product, which is a reasonable assumption as paraffinic compounds are the major products in low-temperature FT-synthesis (LTFT) with cobalt catalysts [72] [73]. Product mole fractions were calculated according to Equation (9) based on $\alpha = 0.85$, which corresponds to a typical chain growth probability of LTFT with cobalt catalyst [42]. Though, the methane yield was adjusted to $w_{n=1} = 0.12$, as it was shown based on the used experimental data that methane production was not well reflected by the ASF distribution [74] [75]. Alkanes from CH_4 to $C_{30}H_{62}$ as well as $C_{32}H_{66}$ and $C_{34}H_{70}$ were considered as products. Operation temperature and pressure were set to 230 °C and 25 bar, respectively, and a per-pass CO conversion of 40 % was assumed [28]. In order to avoid uncontrollable temperature peaks within fix-bed FT reactors, the share of reactants (H_2, CO) in the feed gas was limited to 50 % [42] by adjusting the flow of the internal recycle. Cooling is provided by producing steam in a water jacket operating at 25 bar (evaporation temperature ≈ 224 °C).

Product separation and upgrading

Product recovery is modelled by a number of five serial flashes. In a first step, FT-Syncrude is cooled down to 160 °C. Condensed waxen long hydrocarbons are further processed in a hydrocracker in order to increase the kerosene and diesel yield. The hydrocracker operating at 350 °C and 60 bar is modeled as a yield reactor with a defined product distribution adapted from [76]. The gaseous product stream is further cooled in the following flashes with operating temperatures of 100 °C, 45 °C, 0 °C -30 °C, respectively. Cooling of the last two flashes is provided by refrigeration systems working at evaporation temperatures of -15 °C and -45 °C, respectively. Power demand of both refrigeration systems were estimated based on a realistic COP estimation adapted from [16] (See chapter A in the supplementary information). Gaseous components leaving the last flash consist of unreacted reactants (H_2, CO), light hydrocarbons (mainly CH_4) as well as CO_2 and are reused in the internal and external recycle. Though, around 2 % of the recycle stream is sent to the burner in order to avoid accumulation of trace components such as N_2. The liquid product fraction is expanded to ambient pressure and tail gas is collected and sent to the rWGS burner (PBtL and PtL concept) and gas turbine (BtL concept), respectively. A total pressure drop of $\Delta p = 3$ bar in the FT and separation section was assumed.

Heat integration

Heat integration was carried out by applying the pinch analysis method [18]. Required heating and cooling streams were identified and composite curves were created. Based on the composite curves, heat exchanger networks were designed to minimize external cooling and heating demand. A minimum pinch point temperature of 15 °C, 30 °C and 40 °C was defined for heat exchanger with liquid/liquid, liquid/gas and solely gaseous streams, respectively [17]. Excess waste heat including sensible heat of hot gases and remaining fuel gas is than used to produce electricity (gas turbine in BtL concept, steam turbine in PBtL and PtL concepts) as well as steam at different pressure levels (25 bar and 4 bar) and district heat (100°C, 16 bar). Cooling in the temperature interval 30 °C to 90 °C is realized by using river water at 15 °C. Electricity produced in the BtL concept is used to cover the internal demand. Excess electricity is fed into the local power grid. A summary of assumptions used for the gas and steam turbine process is given in chapter A of the supplementary information.

Definition of efficiencies

The performance of the three concepts was evaluated in terms of the X-to-Liquid and overall plant efficiency as well as the carbon conversion rate, which are defined in *Table 4*. The X-to-Liquid efficiency, determining the conversion efficiency from raw materials/utilities to fuel, comprises of the energy content of the liquid FT-product (LHV) divided by all energy flows entering the system. In contrast, the overall system efficiency also considers the by-products electricity (only in the BtL concept) and useful heat (steam and district heat), which is reasonable in the case that a large heat market exists in the vicinity of the plant (heat case). The carbon conversion defines which share of carbon atoms entering the system with biomass and the CO_2 feed ends up in the liquid fuel product. It is an important measure to evaluate the maximum fuel yield from a given biomass or carbon dioxide potential.

Table 4: Definition of process performance parameters

Name	*Formula*	
X-to-Liquid efficiency	$\eta_{XtL} = \frac{\dot{m}_{PR} \cdot LHV_{PR}}{\dot{m}_{BIOMASS} \cdot LHV_{Biomass} + P_{elec}}$	(11)
Overall plant efficiency	$\eta_{Plant} = \frac{\dot{m}_{PR} \cdot LHV_{PR} + P_{elec,out} + \sum \dot{Q}_{heat}}{\dot{m}_{BIOMASS} \cdot LHV_{Biomass} + P_{elec}}$	(12)
Carbon conversion	$\eta_{C} = \frac{\dot{n}_{C,PR}}{\dot{n}_{C,Biomass} + \dot{n}_{C,CO_2,feed}}$	(13)

3.3 Assumptions for techno-economic evaluation

The techno-economic evaluation was conducted for the base year 2014 with all monetary flows given in €$_{2014}$. It was assumed that the plant operation time is 30 years and that all plants run 8260 full-load hours per year. Data used for estimating equipment costs according to Equations (1) & (2) are summarized in *Table 5*. Old cost data were updated to €$_{2014}$. Cost data of standard equipment such as pumps, compressors and heat exchangers are typically subject to uncertainties in the range between +/- 30 %, whereas equipment costs of new or process specific technologies such as biomass gasifiers, electrolyzers and FT-reactor are characterized by much larger level of uncertainty due to lack of sufficient reference data. It shall be noted that some of the given equipment cost functions are simplified in order to make the data comparable to reference values from scientific literature (see footnotes in *Table 5*). Total capital expenditures were subsequent estimated by applying the ratio factors stated in *Table 1*.

Table 5: Used equipment costs data from TEPET database [1] *Equipment costs in million €*$_{2014}$

	ECref[1]	***Sref***	***Unit***	***d***	***Ref.***
Burner	1.97	20	*MW (heat duty)*	0.83	[7]
Compressor[a]	0.49	413	*kW (power consumption)*	0.68	[7]
Cyclone	0.05	1	m^3*/s (total gas flow)*	0.7	[39]
EF-gasifier	103.65	78	*t/h (slurry input)*	0.7	[34]
Electrolyzer[b]	0.64	1	*MW (installed capacity)*	1	[77]
Evaporator[a,c]	0.93	1000	m^2 *(surface area)*	0.54	[7]
Fast pyrolysis	5.98	14.3	*t/h (biomass input)*	0.7	[34]
Gas/liquid separator[a,d]	0.09	10	*m (unit length)*	0.79	[7]
FT reactor	17.62	208	m^3 *(reactor volume)*	1	[31]
Gas-Turbine cycle	8.47	25	*MW (power output)*	0.7	[30]
Guard beds	0.02	8	m^3*/s (gas flow)*	1	[34]
Heat exchanger[a,e]	0.26	1000	m^2 *(surface area)*	1	[7]
Hydrocracker	7.79	1.13	*kg/s (feed mass flow)*	0.7	[39] [38]
PSA	5.89	0.294	*kmol/s (purge gas flow)*	0.74	[39]
Pump[a,f]	0.1	10	m^3*/s (liquid flow)*	0.36	[7]
Refrigeration system[a,g]	1.06	500	*kW (power consumption)*	0.68	[7]
rWGS reactor	2.4	2556	*t/day (total mass flow)*	0.65	[39] [38]
Selexol unit	59.5	9909	*kmol/h (*CO_2 *in feed)*	0.7	[30]
Steam turbine[a]	0.34	10.5	*MW (power output)*	0.44	[7]
WGS reactor	2.78	150	*kg/s (total gas feed)*	0.67	[78]

[a] Equipment costs include additional material costs (material adjustment factor for stainless steel)

[b] Costs for Instrumentation and control, piping & electrical systems, buildings, services facilities and engineering and construction expenses are already included in the given equipment costs

[c] Cost function with two input parameters (area, pressure). The stated cost function is based on a vertical tube evaporator suitable for pressure level up to 10 bar

[d] Cost data for storage vessels were used. The cost function has three input parameters (vessel length, vessel diameter, pressure). The stated cost function is an example based on a horizontal storage vessel with a diameter of 2 m at pressure levels up to 10 bar

[e] Equipment costs for a flat plate heat exchanger. Data for tube & shell heat exchanger available in the TEPET database

[f] Cost function with two input parameters (flow rate, pressure). The stated cost function characterizes a centrifugal pump suitable for pressure level up to 10 bar

[g] Cost function with two input parameters (capacity, evaporator temperature). The given example describes a refrigeration system with an evaporation temperature of -29 °C

Applied market prices for raw materials and utilities are summarized in *Table 6*. Market prices were already updated to 2014 by applying the World Bank Commodity Price Data (The Pink Sheet). Additional indirect and direct OPEX were calculated based on the ratio factors 1-8 given in *Table 2* for fluid processing chemical plants according to [7]. Though, distribution and selling costs as well as expenses for research and development were neglected, since the pure fuel production costs shall be investigated.

Expenses for maintenance labor and material were predicted to be both 2 % of FCI. Required hours of labor were estimated based on the total product output of the modelled plants and the number of key process steps according to the work of Peters et al. [7] (see chapter B of the supplementary information).

Specific labor costs of $c_{labor} = 37$ €/h were assumed corresponding to typical working costs in the German petrol industry [88].

Table 6: Applied market prices for raw materials, utilities and by-products

Raw material / utility / byproduct	***Market price (2014)***	***Unit***	***Ref.***
Biomass (wet)[a]	97.4	€/t	[79]
Clean water	2	€/m^3	[65]
Cooling water[b]	0.00125	€/m^3	[80]
CO_2	37.75	€/t	[81]
District heat (revenue)	0.04	kWh	[82]
Electricity (from grid)[c]	105	€/MWh	[83]
Electricity (to grid, revenue)[d]	58.5 – 136.6	€/MWh	[84]
Low pressure steam (4 bar)[e]	25.7	€/t	[85]
Medium pressure steam (25 bar)[e]	26.3	€/t	[85]
Oxygen[f]	23.7	€/t	[71]
Selexol[g]	4.4	€/kg	[86]
Waste water[h]	2.5	€/m^3	[87]

[a] Residual moisture = 10 wt%

[b] Cost for cooling water extraction from the Elbe river

[c] Electricity prices for industrial consumers in Germany with annual consumption in the range of >70,000 MWh. Recoverable taxes and levies were not included.

[d] The revenue for exporting electricity in the BtL-concept is calculated based on the guaranteed feed-in tariffs according to the German Renewable Energy Law. The feed-in tariffs for biomass based electricity are defined as follows: first 150 kW→ 13.66 €cent/kWh, up to 500 kW → 11.78 €cent/kWh, up to 5 MW → 10.55 €cent/kWh, up to 20 MW → 5.85 €cent/kWh.

[e] Revenue for selling steam was calculated by multiplying the energy needed to heat up water from 40°C to 150°C (low pressure steam) and 225 °C (medium pressure steam) with the average natural gas price for large industrial customers in Germany 2014 of 8.42 €/GJ [85]. Specific capital costs were assumed with 1 % for low pressure steam and 2 % for medium pressure units.

[f] Oxygen from cryogenic methods based on the year 2013. The price was converted to € and updated to 2014 by using the non-energy index of the World Bank Commodity Price Data (The Pink Sheet).

[g] Selexol solvent cost from 2009. The price was converted to € and updated to 2014 by using the non-energy index of the World Bank Commodity Price Data (The Pink Sheet).

[h] Waste water costs in Germany are typical in the range between 1.5 and 2 €. Slightly higher costs were assumed due to the existence of hydrocarbons in the waste water and the therefore necessary pretreatment.

3.4 Model results

Stream tables of Aspen Plus simulations are available in chapter D of the SI. Main material and energy flows as well as system efficiencies for the four investigated X-to-Liquid concepts are summarized in *Table 7*. Streams consumed in the process have by definition a negative sign. Three characteristic efficiencies namely X-to-Liquid, overall system (including byproducts steam and electricity) and carbon conversion were calculated. Details on efficiency definitions are given in Table 4.

About 2.93 t/h and 11 t/h of liquid fuel are produced from 19.8 t_{dry}/h biomass in the BtL and PBtL concept, respectively. Thus, fuel output of BtL concepts was almost quadruplicated by adding hydrogen to the synthesis. The FT-product has a density of 0.7 kg/l and lower heating value of 44 MJ/kg (30.8 MJ/l). A similar high X-to-Liquid efficiency was estimated for the PBtL and PtL concept, whereas the BtL concept is characterized by a significant lower efficiency. Low temperature in the WGS reactor inhibits methane and ethane conversion into syngas. As a consequence, large quantities of valuable tail gas remain unused reducing the BtL XtL-efficiency. The reverse WGS in the PBtL and PtL design runs at sufficient high temperatures to reform the tail gas completely.

Table 7: Energy flows and performance characteristics of the investigated X-to-Liquid concepts

Material flows [kt/a]	*BtL*	*PBtL*	*PtL (Small/Large)*
Biomass	-181.7	-181.7	-
CO_2	-	-	-74.8 / -282.5
Clean water	-709.9	-900	-252.6 / -953.9
Cooling water	-10,548	-59,713	-12,417 / -46,876
Waste water	780.9	883.4	131.1 / 496.6
Oxygen	-76.1	100.4	83.7 / 316.3
Liquid fuel	24.2	91.3	24.2 / 91.2
Energy flows [MW]			
Electricity	12.4	-164.6	-70.7 / -267.1
Biomass	-98.3	-98.3	0
Steam 25 bar	18.1	20.7	9 / 33.7
Steam 4 bar	1.8	0	0
District heating	13.2	15	2.5 / 9.5
Fuel output	35.7	135.1	35.8/ 134.9
Efficiencies			
X-to-Liquid	***36.3 %***	**51.4 %**	**50.6 %**
Overall plant	***82.6 %***	**65.0 %**	**66.8 %**
Carbon conversion	***24.9 %***	**97.7 %**	**98 %**

Results of heat integration are exemplarily shown for the BtL concept in terms of the composite curves *(Figure 4)* and the final composite curves taking into account steam and heat exports as well as heat exchange with the environment (*Figure 5*). It shall be noted that tail gas and remaining pyrolysis gas are utilized in a gas turbine cycle. The hot turbine exhaust gas is than included in the heat integration. Composite curves for the PBtL and BtL concepts are available in chapter A of the supplementary information.

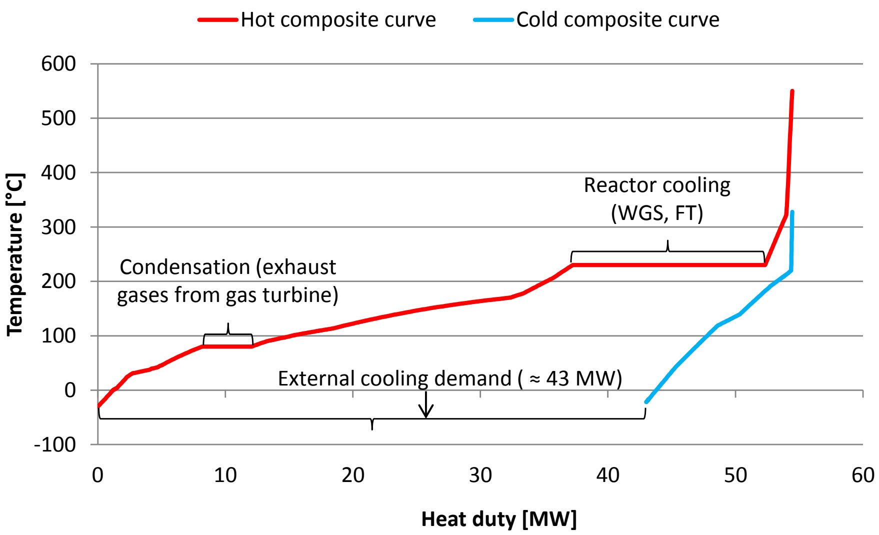

Figure 4: Composite curves of the BtL model

The BtL process is very exothermic with significant isothermal heat integration potentials at 230 °C (WGS and FT-Reactor) and ≈ 80 °C (condensation of off-gases from the gas turbine cycle). The pinch point is located at 320 °C at the end of the cold composite curve. Hence, only external cooling is required. Heat integration reveals a significant potential for the production of steam at 25 bar and 4 bar as well as district heat. A very efficient heat exchanger design was found and implemented as shown in the final composite curve (Figure 5) resulting in an overall plant efficiency of close to 83 %. Results of the heat integration of the PBtL and PtL model in terms of produced steam and district heat are given in Table 7.

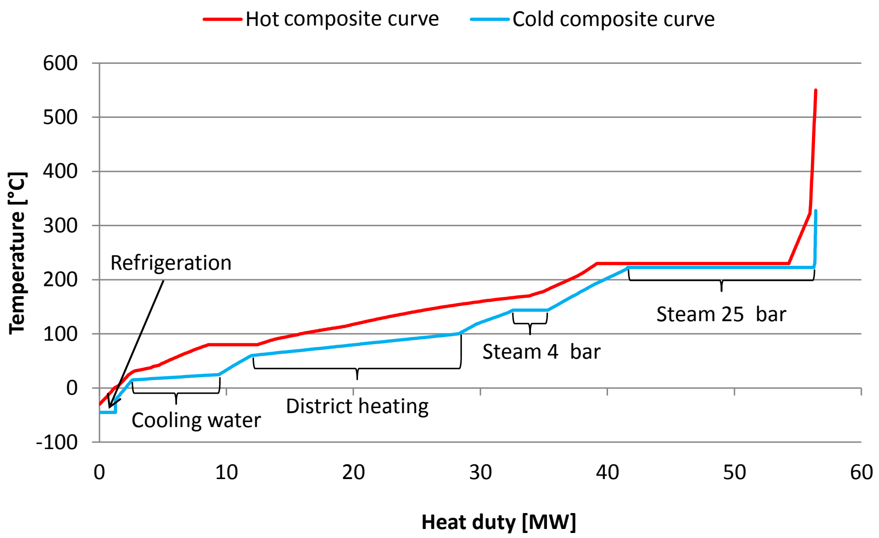

Figure 5: Balanced composite curves after heat integration

The overall plant efficiency of the BtL system is superior compared to the other concepts. This is due to the fact that tail gas and other by-products are already utilized in the burner to cover the high temperature heat demand of the endothermic rWGS reaction in the PBtL and PtL concept, thus reducing the amount of produced steam and district heat. Furthermore, waste heat from PEM electrolysis arises at a temperature below 90 °C offering a negligible heat integration potential.

Carbon is almost completely converted in the PBtL and PtL concepts due to the recycling of CO_2 rich off-gases from the oxy-fuel burner. Minor carbon amounts are lost due to a small required purge stream. In the BtL plant, CO_2 has to be removed before FT-synthesis in the Selexol^{TM} unit. Furthermore, off gases from the gas turbine cannot be further used. Thus, only one quarter of the carbon intricately stored in biomass is converted to precious biofuels.

3.5 Economic results from TEPET

3.5.1 Fuel net production costs (NPC)

TEPET allows the automated calculation of total CAPEX and OPEX directly from process simulation results according to the previous presented methodology. A detailed summary of equipment costs and operational expenditures is provided in chapter E in the supplementary information. Total fuel net production costs for the four investigates X-to-liquid cases are summarized in *Table 8* broken down in CAPEX, direct and indirect OPEX. Thereby, a distinction is made between a standard case assuming that no district heat and steam can be sold and a heat case assuming that all heat can be exported.

Table 8: Fuel net production costs of investigated X-to-Liquid concepts

X-to-Liquid concept		*BtL*	*PtL*	*PBtL*	*PtL*
Plant capacity	*[t/h]*	*2.9*	*2.9*	*11*	*11*
CAPEX	[€/l_{GE}][a]	0.95	0.46	0.48	0.43
Direct OPEX	[€/l_{GE}]	0.45	1.90	1.29	1.90
Indirect OPEX	[€/l_{GE}]	0.94	0.49	0.47	0.41
NPC	**[€/l_{GE}]**	**2.34**	**2.85**	**2.24**	**2.74**
NPC (heat case)	[€/l_{GE}]	2.05	2.75	2.15	2.64

[a] GE = Gasoline equivalent based on a typical energy density of gasoline of 32 MJ/l. Thus, one liter of FT-product has the same energy content as 0.96 l of standard gasoline.

Figure 6 shows a detailed breakdown of NPC for the case without heat market. NPC rises from the PBtL to the BtL plant and further to the large and small scale PtL plant, as shown in *Figure 6*. The poor performance of the PtL plants is primarily due to the high expenses for raw materials and utilities (direct OPEX), which accounts for approximately 67 % of total fuel costs. Purchase costs for electricity are by far the largest cost factor both in the PBtL and PtL concept. Lower electricity demand in the PBtL plant due to utilization of high energy syngas from biomass gasification explains the lower specific direct OPEX. Expenses on other raw materials such as CO_2 and biomass seem to be negligible.

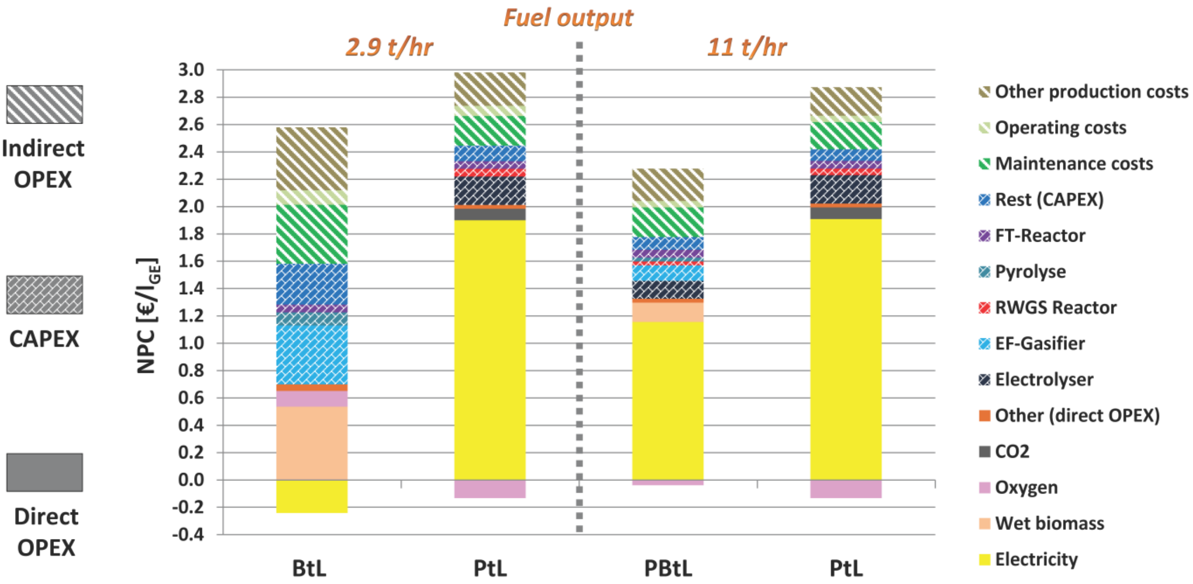

Figure 6: Fuel net production costs broken down by mayor cost factors

Although CAPEX of the PEM electrolysis unit accounts for more than 60 % of total CAPEX costs in the PtL cases, the total share on the fuel production costs is less than 8 %. The same applies for the PBtL plant, where electrolyzer and gasifier together make up 60 % of CAPEX. On the contrary, the BtL plant is characterized by a different cost structure, where direct OPEX accounts for only 20 % and CAPEX for around 37 % of the fuel price. Capital costs for the gasifier are the second largest cost factor behind biomass costs accounting for approximately 18 % of the total fuel production costs. Taking into account revenues from heat sale (heat case), NPC was slightly reduced by 9-10 €ct/l and 29 €ct/l in the PBtL/PtL and BtL concepts, respectively. This indicates that a local heat market offers a low cost reduction potential below 4 % for PBtL and PtL plants, whereas heat sales significantly reduce NPC in the BtL case.

3.5.2 Local sensitivity analysis

TEPET was used to identify sensible cost factors. For this purpose, more than 100 economic parameters were varied in a local sensitivity analysis within a range between -70 % and + 70 % of its initial value. Results of the three most important cost factors are presented in *Figure 7*.

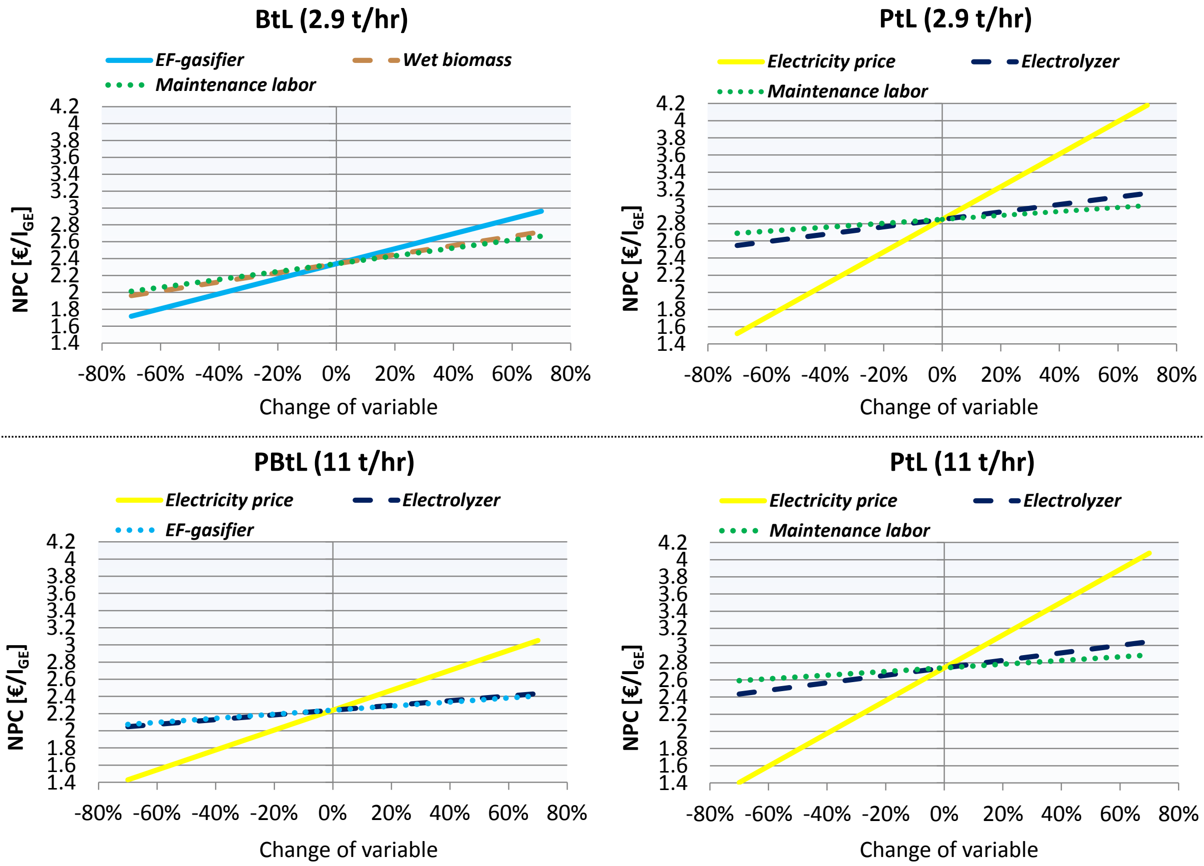

Figure 7: Results of sensitivity analysis

Electricity price has by far the most significant impact on NPC in the PBtL and PtL concepts, confirming the results of König et al. [22]. The second and third most sensitive cost factors (capital costs for electrolyzer, gasifier (PBtL) and maintenance labor costs (PtL)) have a much smaller effect on NPC. Lower power prices can be assumed for a PtL plant close to a large (renewable) power generation unit, e.g. a wind farm or a hydroelectric power station. Hence, grid fees, taxes and other additional costs may be neglected and the average market price of electricity traded at the Europe Energy Exchange (EEX) [89] of 32.8 €/MWh in the year 2014 may be more realistic (see next subsection).

Capital costs for the gasifier are the most sensible BtL cost factor, followed by the biomass price and maintenance labor costs. A 70 % reduction of gasifier purchased costs results in 26 % lower fuel production costs of 1.72 €/l_{GE}. This highlights the continuous gasifier research need.

3.5.3 Economy of scale vs. electricity price

The investigated X-to-Liquid plant capacity in this work was defined due to the predicted biomass potential. In order to account for scale effects, the net fuel production costs were estimated as a function of both plant capacity and electricity price with TEPET. Plant capacity and electricity price were varied in the range between 25-240 kt/year and 20-105 €/MWh, respectively. NPC were assigned to each combination of plant capacity and electricity costs resulting in a surface plot for each of the three concepts. All three surface plots were superimposed and only the lowest NPC for every coordinate was considered. The results are illustrated in *Figure 8*.

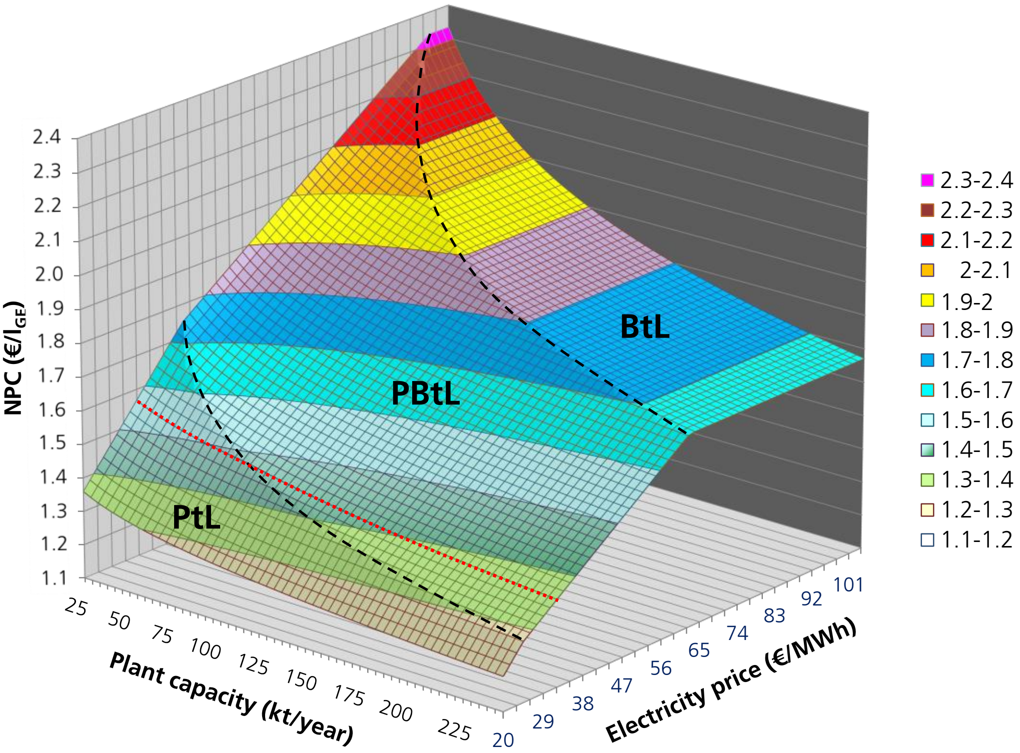

Figure 8: NPC as a function of plant capacity and electricity price

Economy of scale affects the capital investment costs as well as labor and maintenance costs resulting in considerable lower NPC for larger production plants. The envelope curve can be divided into three areas, where every of the three investigated concepts is superior to the others in terms of lowest NPC.

NPC of BtL plants is not dependent on electricity prices, since no external electricity source is needed. Thus, the BtL concept is favorable at high electricity prices independent of the plant scale. However, one shall keep in mind that plant capacity is strictly limited by the biomass availability. With decreasing power costs, the higher system efficiency along with increased carbon conversion results in lowest production costs in the PBtL concept. The PtL concept is superior at power costs below approximately 38 €/MW and biomass cost at 97.4 €/t_{wet} reaching fuel production costs below 1.40 €/l_{GE} for large PtL plants. The slope of the envelope curve with regards to the power costs is steepest for the PtL concept.

Figure 8 indicates the most economic feasible concept due to any given electricity price at fixed biomass cost. At an electricity price of 32.8 €/MWh (EEX Phelix marked as dotted red line in *Figure 8*), the PtL concept is favorable for small scale plants with an annual fuel output up to 70 kt/year, whereas PBtL plants are more profitable for plants with larger fuel output.

3.5.4 Comparison with scientific literature

Results of previous techno-economic studies on BtL Fischer-Tropsch concepts have already been compared in detail by Haarlemmer et al. [12]. Relevant studies had been normalized, as far as possible, to a plant capacity of 400 MW_{th} (LHV biomass) and cost data was updated to $€_{2011}$. CAPEX between 300 and 1100 M€ and fuel production costs in the range of 0.80-1.65 $€_{2011}$/l were reported for the 2σ interval (95.8 % of all studies), though, the authors expected realistic results to be closer to the upper limit. When scaling results of this study in the same way, CAPEX of 990 and 995 $M€_{2014}$ along with NPC of 1.75 and 1.40 $€_{2014}$/l were estimated for the base case and heat case, respectively. It shall be noted that the currency basis is still $€_{2014}$ and that NPC will be slightly lower in a $€_{2011}$ calculation. In general, results are within the typical range, though, closer to the upper limit of the ranges given for CAPEX and NPC.

Only a few studies have so far been published on PtL and PBtL Fischer-Tropsch concepts. Becker et al. [38] reported NPC between 0.83 and 2.83 $€_{2009}$/l_{GE} for a SOEC PtL plant (Electricity input 54.4 MW) based on various electricity prices (range: 0-105 $€_{2009}$/kWh), capacity factors (range: 40-90 %) and CO conversion rates in the FT reactor (range: 70-90 %). Applying the particular assumptions used in this work results in NPC of approximately 2.56 $€_{2014}/l_{GE}$. This is in good agreement with the results presented in the case study. The slightly lower NPC arises first of all due to lower assumed specific electrolyzer costs of around 300 $€_{2014}/kW_{installed\_capacity}$. König et al. [22] reported NPC of 3.39 $€_{2014}/l_{GE}$ for a 1.5 $GW_{electrical}$ PEM PTL plant running on green electricity (140 €/MWh). When recalculating NPC with a power price of 105€/MWh, NPC is reduced to 2.77 $€_{2014}/l_{GE}$, which is in line with our results.

Baliban et al. [41] published a techno-economic study on a 780 t/day PBtL FT plant assuming different electricity prices in the range between 25-70 €/MWh. No fuel net production costs were reported, but it was stated that economic feasibility is reached at a break even crude oil price between 100 and 150 $\$_{2010}$/bbl. However, a reasonable value for NPC cannot be derived from the given information.

Seiler et al. [43] estimated NPC of 0.95 $€_{2010}/l$ for a PBtL FT plant with a capacity of 1.43 GW_{th} (LHV biomass ≈ 300 t_{dry}/h) and electricity costs of 45 €/MWh. The amount of hydrogen added prior to the FT-synthesis as well as capital costs of the gasifier and electrolyzer are not included in the paper. Recalculating NPC considering the same capacity and electricity price results in NPC of 1.29 $€_{2014}/l$ for this study. The reasons for the discrepancy cannot be given due to a lack of information on the cost calculation methodology in the reference paper.

3.6 Summary of results

An X-to-Liquid efficiency of 36.3 %, 51.4 % and 50.6 % was estimated for the BtL, PBtL and PtL plant, respectively. Predicting an unlimited heat market, overall system efficiency up to 82 % can be obtained. Though, selling steam and district heat result in only slightly lower fuel costs. Carbon conversion rates close to 98 % were achieved in the PBtL and PtL plant by using oxy-fuel technology and recycling tail gas and exhaust gases in the rWGS reactor. With a biomass supply of 181.6 kt/a, about 24 kt/a and 91 kt/a of renewable fuel can be produced with the BtL and PBtL concept, respectively. Hence, fuel output was increased by a factor of 3.75 in the PBtL plant. Assuming an electricity price of 105 €/MWh, fuel net production costs from 2.24 €/l to 2.81 €/l were calculated, whereby the PBtL concept is characterized by the lowest NPC. All fuel production costs are significant higher compared to fossil reference fuels. High direct OPEX diminish the economy of scale effect on NPC of PBtL and PtL plants with fuel outputs larger than 20 kt/a. On the contrary, CAPEX and indirect OPEX make up 80 % of NPC in the BtL concept. Thus, up-scaling of a BtL plant is attractive from an economic point of view, although plant capacity is typically limited by the local biomass availability.

3.7 Discussion

With the exception of the electrolyzer and the rWGS reactor, all X-to-Liquid concepts are based on standard available technologies. Though, the applied cost data is subject to uncertainty due to a lack of pilot plants and experience with green FT-plants. Furthermore, capital costs of novel technologies are hard to predict, since experience curve effects are often unknown. The same applies for ratio factors adapted from best practice estimates from the chemical industry, which are used in the case study to estimate indirect costs such as maintenance and installation costs as a fraction of fixed capital investment. This bears the risk to overestimate indirect costs, since capital costs of novel technologies are significantly higher compared to standard equipment used in state-of-the-art chemical processes. More research is required to estimate realistic cost factors for novel fuel production processes.

The implemented flowsheet models of the BtL, PBtL and PtL concepts comprise of all key process steps required for the production of green FT-fuels. However, some auxiliary systems such as the refrigeration systems or the CO_2 capture unit were handled as a black box or even neglected such as biomass pre-drying. It shall be noted that a further optimization potential for heat integration exists when including these devices in the flowsheet models, especially, since results from the case study show that all concepts are characterized by a great surplus of heat. Further optimization potentials regarding auxiliary systems as well as promising process alternatives (e.g. hot gas cleaning, hot-temperature electrolysis SOEC) will be investigated at a later stage in terms of an exergoeconomic optimization in order to identify the most economic feasible process designs.

4 Conclusion

The presented standardized methodology for the techno-economic analysis with the software-tool TEPET enables the assessment of different alternative fuel production concepts based on similar technical and economic assumptions and boundary conditions. Results can be used to identify weaknesses and strengths of each concept. Furthermore, economic cost saving potential can be quantified. As a consequence, the methodology allows process optimization from an economic point of view. The results can be used within political and commercial decision making processes to identify appropriate technical solutions for given boundary conditions.

Results from the case study indicate that electricity price is the largest cost driver and most sensible cost factor in both the PBtL and PtL FT concept. Significant lower electricity prices neglecting grid fees, taxes and other transmission costs results in lower and more competitive NPC below 1.40 €/l_{GE}. Capital costs for the biomass gasifier are the most sensible cost factor in the BtL concept. The results from techno-economic evaluation can be used to identify the most cost efficient plant concept for a given plant capacity and electricity price. Calculated fuel net production costs correspond with results of previous published techno-economic studies on BtL, PtL and PBtL concepts.

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ABBREVIATIONS

ACC	Annualized capital cost
ASF	Anderson-Schulz-Flory distribution
BtL	Biomass-to-Liquid
CAPEX	Capital expenditures
CEA	Commissariat à l’énergie atomique et aux énergies alternatives
CEPCI	Chemical Engineering Plant Cost Index
CPI	Commodity price index
CtL	Coal-to-Liquid
DME	Dimethyl Ether
EC	Equipment costs
EEX	European Energy Exchange
FCI	Fixed capital investment
FT	Fischer-Tropsch
GE	Gasoline equivalent
GHG	Greenhouse gas
GtL	Gas-to-Liquid
HEFA	Hydro-processed esters and fatty acids
HTFT	High-temperature Fischer-Tropsch
IR	Interest rate (%)
KIT	Karlsruhe Institute of Technology
LTFT	Low-temperature Fischer-Tropsch
LHV	Lower heating value
MtG	Methanol-to-Gasoline
NPC	Net production costs
NREL	National Renewable Energy Laboratory
OL	Operating labor
OPEX	Operational expenditures
PBtL	Power and Biomass-to-Liquid
PEM	Proton exchange membrane
PO	Plant overhead costs
PSA	Pressure swing adsorption
PtL	Power-to-Liquid
rWGS	Reverse water gas shift
SI	Supplementary information
SOEC	Solid oxide electrolyzer cell
TCI	Total capital investment
TEE	Techno-economic evaluation
VTT	Technical Research Centre of Finland

GREEK LETTERS & VARIABLES

α	Chain growth probability
ρ	Density (kg/m^3)
ω	Energy density (MJ/l)
γ_{BM}	Biomass yield (t/(km^2 year))
η_C	Carbon conversion
η_{Plant}	Overall plant efficiency
η_{XtL}	X-to-Liquid efficiency

c	Cost of raw materials, utilities, power, heat
cf_{plant}	Capacity factor of X-to-Liquid plant
c_{labor}	Labor costs (€/h)
d_i	Digression factor of unit i
E_{power}	Power consumption/production (MWh)
f_i	Equipment cost function of unit i
F_{eco}	Ratio factors for estimating FCI
F_{mat}	Multiplier for material related equipment costs
F_{pre}	Multiplier for pressure related equipment costs
h_{labor}	Total working hours
ΔH_R^0	Standard enthalpy of reaction (kJ/mol)
i,k,m,o	Control variables
L_i	Learning rate of unit i
$\dot{m}$	Mass flow (t/h)
n	Number of produced units
p	Pressure (bar)
P	Power (MW)
r	Radius (km)
$S_{i,k}$	kth input variable of cost function of unit i
T	Temperature (°C)
W	Heat export (MWh)
w	Mass fraction
x	Molar fraction
y	plant operation time (years)

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