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Life cycle assessment-based guidance for development of new energy technologies

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Citation

Giesen, C. C. van der. (2020, October 27). *Life cycle assessment-based guidance for development of new energy technologies*. Retrieved from <https://hdl.handle.net/1887/137930>

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Title: Life cycle assessment-based guidance for development of new energy technologies

Issue date: 2020-10-27

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Chapter 3

Energy and Climate Impacts of Producing Synthetic Hydrocarbon Fuels from CO₂

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Re-print from:
Environmental Science & Technology (2014) 48: 7111-7121.
doi/10.1021/es500191g

Abstract

Within the context of carbon dioxide (CO_2) utilization there is an increasing interest in using CO_2 as a resource to produce sustainable liquid hydrocarbon fuels. When these fuels are produced by solely using solar energy they are labelled as solar fuels. In the recent discourse on solar fuels intuitive arguments are used to support the prospects of these fuels. This paper takes a quantitative approach to investigate some of the claims made in this discussion. We analyse the life cycle performance of various classes of solar fuel processes using different primary energy and CO_2 sources. We compare their efficacy with respect to carbon mitigation with ubiquitous fossil-based fuels and conclude that producing liquid hydrocarbon fuels starting from CO_2 by using existing technologies requires much more energy than existing fuels. An improvement in life cycle CO_2 emissions is only found when solar energy and atmospheric CO_2 are used. Producing fuels from CO_2 is a very long term niche at best, not the panacea suggested in the recent public discourse.

3.1 Introduction

There is an increasing interest in the use of carbon dioxide (CO₂) as a resource. The recent introduction of the Journal of CO₂ Utilization and conferences like the Carbon Utilization Summit 2013 (Carbon Utilization Summit 2013 2013), the International Conference on CO₂ Utilization (ICCDU XII 2013 2013) and the 2nd Conference on CO₂ (Nova-Institut GmbH 2013) testify to this. These platforms make the case for (more) research on the conversion of CO₂ into synthetic fuels as means to utilize CO₂ and thereby mitigate its accumulation in the atmosphere. As such it is presented as a useful addition to, or alternative for geological sequestration, offering the prospects of ‘productive use’ and or ‘recycling’ as opposed to mere (unproductive, unprofitable) ‘storage’. In this spirit, the Global CCS institute initiated a study to investigate possible uses of CO₂ to accelerate the development and commercial deployment of carbon capture and sequestration (CCS) (Global CCS institute and Parsons Brinckerhoff 2011). One of its conclusions is that, once technically mature, producing liquid hydrocarbon fuels from CO₂ might be a promising driver for the development of carbon capture.

In this paper we assess the environmental merits of synthetic liquid hydrocarbon fuels produced from CO₂ compared to alternative fuel production routes. When the required energy for the production of these fuels is taken from the sun, these fuels are also labelled as “solar fuels”. This term is at present loosely defined and is applied to a wide variety of sustainable energy pathways, encompassing anything from solar power, solar hydrogen, algal fuels, next-generation biofuels to synthetic fuels from CO₂ using either conventional chemical processes or yet-to-be-invented ‘artificial leaves’ (Nocera 2012). This ambiguity in definition allows for the opportunistic use of sustainability arguments. It also suggests both a sweeping future scope of solar fuels as a class, as well as having both short-, medium- and long-term prospects while the implied breadth makes it difficult to quantify metrics of success. The following question has been neglected so far: what is success? Under what conditions is a ‘solar fuel’ better than (a combination of) existing processes? For instance: is recycling CO₂ from a coal power plant into a synthetic fuel with hydrogen generated from renewable energy sources preferable over the direct displacement (phase-out) of coal by that same renewable power and the (continued) use fossil-based liquid fuel?

For this purpose we define solar fuels as liquid hydrocarbon fuels produced from CO₂, water and solar energy. This is a narrower definition than others that might include solar hydrogen or even solar electricity. Since solar electricity or more broadly renewable electricity is an established and well-described branch of technology, we propose not to include it in a new fuzzy term, as long as we have not explicitly established the merit of so doing. The same goes for the production of hydrogen from renewable sources. Hydrogen

production – via natural gas steam reforming or via alkaline electrolysis – is established technology, and hydrogen has an existing brand-name of its own as a renewable fuel. This leaves us with ‘solar fuels’ as the umbrella term to describe hydrocarbon fuels produced from CO₂ with renewable energy inputs. A solar fuels process can thus be anything contained in a ‘box’ that has CO₂, water and renewable energy going in, and hydrocarbons coming out. The only ambiguity this leaves is with respect to biofuels. We go forward mindful of that and exclude conventional biofuels from the term (for the same reasons cited above for renewable electricity and hydrogen), but have the term cover (advanced) algal biofuels and other, even more advanced bio-routes, eventually leading to the elusive ‘artificial leaf’.

Scientific research in the field of fuel production from CO₂ mainly focuses on specific techniques to convert CO₂ into hydrocarbon fuels. The most common of these techniques are thermochemical and electro-catalytic approaches and the development of new and improved catalysts to convert hydrogen and CO₂ into synthetic fuels (Romero and Steinfeld 2012; Centi and Perathoner 2010; Roy et al. 2010; Inglis et al. 2012; McDaniel et al. 2013; Woolerton et al. 2012; Tran et al. 2012; Haije and Geerlings 2011; Stechel and Miller 2013; Goeppert et al. 2012; Ampelli et al. 2010). Solar fuels can be produced with a solar-to-fuel efficiency of 10% by using existing technologies (Haije and Geerlings 2011). This efficiency is also suggested as a reasonable minimum goal for research and development for solar fuels (Stechel and Miller 2013).

To contextualize our analysis in the subsequent sections, we first present a structured overview of the arguments that we find in the current public discourse to substantiate the desirability or the need for ‘solar fuels’. We identify four discrete arguments.

Firstly, solar fuels are considered to contribute to a sustainable energy future because they are renewable (hydrocarbon) fuels that can be used in our existing energy infrastructure. This is the same argument that drives the development of biofuels. There can be no doubt that hydrocarbons have properties that make them highly desirable and virtually irreplaceable in certain end-use sectors, notably heavy-duty transport and aviation. Solar fuels offer the promise of enhancing the scope of renewable fuels beyond biofuels. If biofuels now rely by necessity on photosynthesis, a solar fuels process (in our hypothetical ‘box’) would have the same functional use (CO₂, water and renewable energy in; fuel out), but would be driven by a process other than (natural) photosynthesis. This raises two questions: is the solar fuels process better than the incumbents? And: Are solar fuels easier, cheaper or otherwise more attractive than a shift away from hydrocarbon fuels, to hydrogen or electricity?

Secondly, – more intuitive in character – is the argument that solar fuels provide a synergistic solution to the problem of overabundance of CO₂ and the abundance of renewable energy on the one hand, and the scarcity of hydrocarbon fuels on the other. It follows that producing the latter from the former must be inherently attractive (Goeppert et al. 2012; Olah et al. 2011; Keith 2009; Lackner 2009). But is CO₂ really abundantly available? It is abundant only in diluted form, and it takes effort to make it available as a practical feedstock (Roy et al. 2010). And how does the release of CO₂ upon combustion of the solar fuel compromise its value proposition, especially if the CO₂ is of fossil origin? It delays rather than avoids the release of CO₂ into the atmosphere, which is why some – but by no means all – proponents stress that atmospheric CO₂ should be used to produce solar fuels (Stechel and Miller 2013; Goeppert et al. 2012; Olah et al. 2011; Wang 2012; Graves et al. 2011). This study investigates to what extent using CO₂ from a specific source makes a difference to solar fuels' claimed carbon neutrality and also takes into account additional system related GHG emissions.

Thirdly, solar fuels offer the promise of solar energy storage – arguably one of the biggest challenges in a world predominantly relying on renewables (Romero and Steinfeld 2012; Roy et al. 2010; Haije and Geerlings 2011; Gray 2009). The world needs scalable energy storage solutions. But for this solar fuels need to outperform other (existing) energy storage options such as batteries or hydrogen storage, of which the latter is excluded from our solar fuels definition. These options are equally suited for renewables matching, have no a priori limit to scale and are likely to have higher round-trip efficiencies than solar fuels. Moreover, for the production of solar fuels using existing technologies, it can be expected that a continuous process with a continuous resource supply provides the best means of production. A continuous supply of renewable energy is simply not possible, unless one of the previous mentioned energy storage technologies is used.

Finally there is the claim that the costs of carbon capture can be offset by producing valuable fuels or chemical products (CO₂ as a feedstock for chemicals is another strand of recent research activity. Many of the problems/issues are similar to those of solar fuels. We merely note this, while staying focused in this paper on fuel production) from CO₂ which is inherently more financially attractive than storing it underground (Global CCS institute and Parsons Brinckerhoff 2011). But is it? The aim of sequestering CO₂ underground is to prevent its accumulation in the atmosphere while all fuels are eventually combusted, releasing the painstakingly captured CO₂ once again into the atmosphere. Although a possible profit can be made by producing and selling fuels, this argument completely abandons the primary aim of carbon sequestration.

If we review these four broad claim areas, we observe that all of them have merit in principle, but all of them call forth immediate questions of utility. These questions often cannot be answered in abstracto but will require some form of (quantitative) life cycle assessment (LCA). Although the importance of a life cycle approach for these questions has been acknowledged (von der Assen et al. 2013, 2014), the authors are not aware of any existing LCA studies on CO₂ utilization. It has been the observation of the authors that – in the absence of such evidence – the participants in the public and scientific discourse on solar fuels use any or all of the four claims above to substantiate their argument. In the absence of quantitative evidence for or against, four intuitively persuasive arguments make a very strong case indeed. This is the state of affairs as we perceive it to be. It is the purpose of this paper to hold the claims up to quantitative scrutiny and review the general merit of the idea of solar fuels – subject to the definition above.

Here we question if the production of liquid hydrocarbon fuels from CO₂ using existing technologies leads to lower life cycle greenhouse gas emissions and cumulative energy demands than existing liquid fuel routes and aim to answer this question by performing a life cycle assessment (LCA). First the required technologies are identified and possible production routes are described based on the origin of the energy and CO₂ that is used. Then the required processes and technologies are described in such detail that the LCA model can be constructed. Third, the total greenhouse gas emissions and cumulative energy demand are assessed and compared to existing liquid fuel routes. We close by discussing the results and possible implications.

3.2 Research scope and approach

The scope of this study concerns a hypothetical fuel production system that converts CO₂ into liquid hydrocarbon fuels using proven technologies. In this study fuels produced in this way are labelled as synthetic fuels, where the route that uses solar energy is considered to produce solar fuels. Because the system is ultimately intended to be solar energy based it is assumed to be located in Spain, thereby specifying the use of life cycle inventory (LCI) data for this geographical area.

Figure 3.1 shows an overview of two possible system layouts to produce liquid hydrocarbon fuels from CO₂. Fischer-Tropsch (FT) technology is used to convert a combination of CO and hydrogen, called syngas, into synthetic liquid hydrocarbon fuels. CO can be obtained from CO₂ via the reversed water gas shift (RWGS) reaction and hydrogen is produced via water electrolysis. The required CO₂ is obtained from fossil fuelled power plants or directly from the atmosphere. When natural gas or biomass

are combusted, it is assumed that all CO₂ and energy from this process will be used to produce liquid hydrocarbon fuels. Additional electricity supply is required to produce sufficient hydrogen to convert all CO₂ into liquid fuel. In the case of using CO₂ from the atmosphere, all required electricity is generated by PV.

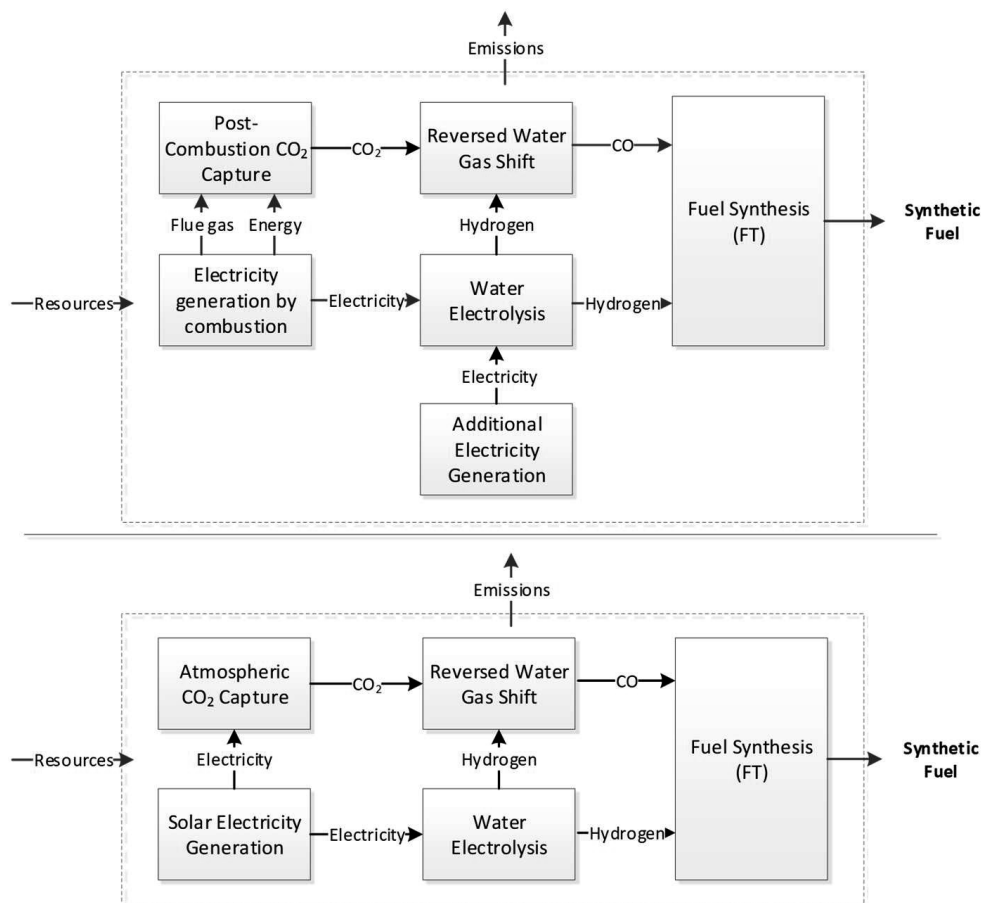


Figure 3.1: Fuel production from fuel combustion based energy and CO₂ (top) and from atmospheric CO₂ using solar electricity (bottom).

Based on three possible CO₂ sources and three energy sources, nine fuel production routes are defined of which five are assessed (see Table 3.1). The NGNG and BMBM alternative are implausible since they provide a very inefficient route to convert natural gas and biomass into liquid fuels. The preferred and currently applied route for this is gas to liquids (GTL) or biomass to liquids (BTL) technology, both of which are based on gasification. However, in this analysis we focus on the conversion of CO₂ to liquid fuels,

therefore we have chosen to include the NGNG and BMBM routes but we have also added GTL and BTL as reference technologies. The assessment of hybrid alternatives like NGBM and BMNG is excluded because these are not fundamentally different in system layout, causing the outcomes to be within the range of the outcomes for NGNG and BMPV. Combining direct air capture (DAC) with electricity from natural gas or biomass combustion (DACNG or DACBM) is also not fundamentally different from the alternatives already assessed. Where NGNG introduces extra CO₂ emissions connected to the use of additional electricity generation, a DACNG system will emit CO₂ emissions in the same range because only part of the total emissions related to the electricity generated will be captured to be converted into a liquid fuel.

The proposed fuel production routes are assessed through LCA with a main focus on the energy and material inputs. The assessment uses fuel production from source-to-fuel expressed in 1 MJ of liquid fuel as functional unit and since the function of a fuel is to deliver energy through combustion, the CO₂ emissions from combustion are also taken into account when calculating net GHG emissions. The outcomes are compared to the performance of existing hydrocarbon fuels like diesel, bio-ethanol from sugar cane, GTL and BTL diesel. For fair comparison pure ethanol is considered. Where possible the ecoinvent 2.2. database (Swiss Centre for Life Cycle Inventories 2010) was used to provide LCI data for the alternatives. Data for GTL and BTL diesel were taken from the GREET (Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation) model (Elgowainy et al. 2012). CMLCA software version 5.2 (Institute of Environmental Sciences) was used to model the different fuel production routes. The following paragraphs describe the main characteristics of all processes and related assumptions from fuel combustion to CO₂ capture (also see the supporting information).

Table 3.1: Different fuel production routes based on CO₂ and energy sources.

	Electricity from natural gas (NG) combustion	Electricity from biomass (BM) combustion	Electricity from PV
CO ₂ from natural gas (NG) combustion	NGNG NG power plant with carbon capture supplies all required CO ₂ and 65% of the energy required to generate sufficient H ₂ to convert all CO ₂ . The additional 35% required energy is supplied by a NG power plant without carbon	NGBM Not assessed	NGPV NG power plant with carbon capture supplies all required CO ₂ and 65% of the energy required to generate sufficient H ₂ to convert all CO ₂ . The additional 35% required energy is supplied by PV electricity generation
CO ₂ from biomass (BM) combustion	BMNG Not assessed	BMBM BM power plant with carbon capture supplies all required CO ₂ and 10% of the energy required to generate sufficient H ₂ to convert all CO ₂ . The additional 90% required energy is supplied by a BM power plant without carbon capture	BMPV BM power plant with carbon capture supplies all required CO ₂ and 10% of the energy required to generate sufficient H ₂ to convert all CO ₂ . The additional 90% required energy is supplied by PV electricity generation
CO ₂ from direct air capture (DAC)	NGDAC Not assessed	BMDAC Not assessed	DACPv CO ₂ is supplied via direct air capture and PV electricity (100%) is used to power this process and supply sufficient hydrogen

*acronyms are based on CO₂ source followed by electricity source. NG = natural gas combustion, BM = biomass combustion, PV = photovoltaic electricity, DAC = direct air capture.

Final fuel combustion

It is assumed that all produced fuels are transported and combusted in a highly comparable manner and that the environmental impacts connected to this part of the life cycle (from gate to end use) do not need to be taken into account. However, since carbon neutrality is an important claim connected to the sustainability of fuels produced from CO₂ this study calculates the GHG balance and takes the hypothetical CO₂ emissions from fuel combustion explicitly into account. It is assumed that GTL and BTL diesel as well as FT diesel have properties comparable to conventional diesel, that is a lower heating value of 43,3 MJ / kg and 0,0716 kg CO₂ emission per MJ fuel combusted (Jungbluth 2007; National Institute of Standards and Technology). For ethanol these numbers are 26,8 MJ / kg and 0,0714 kg CO₂ / MJ (Jungbluth, N., Chudacoff, M., Dauriat, A., Dinkel, F., Doka, G., Faist Emmenegger, M., Gnansounou, E., Kljun, N., Schleiss, K., Spielmann, M., Stettler, C., Sutter 2007).

Fischer - Tropsch process

Fischer-Tropsch (FT) technology is commercially deployed to convert syngas, a 2 : 1 molar ratio mixture of hydrogen and carbon monoxide into liquid hydrocarbon fuels (Haije and Geerlings 2011; Olah et al. 2011; Graves et al. 2011; Eilers et al. 1990). Currently Shell uses the FT technology in their gas-to-liquids (GTL) plant in Qatar where natural gas is converted into syngas (by gasification) which is subsequently converted into liquid fuel. We use the basic performance data of the Shell plant to model the synthesis step in the fuel production processes below, and assume that the straight-run product is equivalent to conventional diesel.

Based on common operating parameters (Eilers et al. 1990; Reinalda 2013) we state the FT reaction to take place at 25 bars (for which both CO₂ and hydrogen are supplied at 25 bar pressure) and a temperature of 230°C with an efficiency of 80%, meaning that 80% of the energy available in the syngas is transferred into fuel. The remaining 20% consists of hydrocarbon chains that are too short to convert into fuels but are sufficient to generate energy to run the GTL plant (Reinalda 2013). The production capacity of this plant is 140.000 barrels of GTL fuel per day, with an average heating value of 43,2 MJ / kg. The process uses 2,3 kg syngas to produce 1 kg of GTL fuel.

Reversed Water Gas Shift (RWGS) reaction

The RWGS reaction is used to produce carbon monoxide (CO) that is blended with hydrogen to form syngas. It is an endothermic equilibrium reaction that uses part of the excess heat produced in the Fischer-Tropsch process for sorbent regeneration (Haije and Geerlings 2011; Reinalda 2013; Haije 2013). Experimental results have shown that CO can be produced from CO₂ and H₂ in a fixed bed reactor which contains a mixture of a

WGS catalyst and a water sorbent. A large scale RWGS reactor has not been constructed until now but could be made available in the short term (Geerlings 2013). Here it is assumed that the RWGS reaction takes place at 230°C / 25 bar and uses 1,57 kg of Carbon dioxide and 0,07 kg of hydrogen to produce 1 kg of carbon monoxide.

Hydrogen production

Hydrogen is commonly produced from natural gas by steam methane reforming (SMR), a process that also emits CO₂. In order not to increase the total system CO₂ emissions further we consider the production of hydrogen through water electrolysis using the electricity from the power plant from which the CO₂ is captured. In the supplementary information an alternative route that uses hydrogen and CO₂ from SMR to produce liquid fuels is discussed. The results of that route are highly comparable to the natural gas based alternatives presented below and are there for not presented in the results section.

The most evolved and widely used water electrolyzing process uses an alkaline electrolyte, typically potassium hydroxide (KOH) which can be retrieved and reused in the process (Tributsch 2008; Pagliaro, M. Konstandopoulos et al. 2010; Kruse et al. 2002; Ivy 2004). Based on standard operating parameters (see section 3.5) the production of 1 kg of hydrogen needs 11 kg of water and uses 56.7 kWh of electricity. An additional amount of 0.66 kWh electricity is needed to compress the hydrogen to 25 bar, which is needed for the downstream processes (Rovers 2005; Sumner 2006).

CO₂ and electricity from fossil fuel combustion

Natural gas or biomass combustion in a power plant with post-combustion carbon capture using monoethanolamine (MEA) provides CO₂ and electricity. Typically only 90% of the CO₂ present in the flue gases is captured, the remaining 10% is emitted into the atmosphere. Because CO₂ and electricity from this power plant are completely used up in the production of FT fuels, there is no need to specifically allocate or assign environmental interventions to electricity or carbon dioxide both produced by the power plant. The required additional electricity to produce sufficient hydrogen to convert all CO₂ into liquid fuel is either generated by an additional power plant without carbon capture running on the same fuel or by PV electricity. PV electricity data is directly taken from the ecoinvent life cycle inventory database (Jungbluth et al. 2007).

Here we assume that a general coal fired power plant with carbon capture can be used for the combustion of biomass as well. When equipped with carbon capture, the energy output from power plants decreases as a result of the energy needed for the carbon capture and compressing the CO₂ to a pressure at which it can be transported. The

energy penalties are dealt with by decreasing the output of energy produced by the power plants, while using the same quantity of fuel input (and related CO₂ emissions). The energy penalties for natural gas and biomass in this study are set at 15% (Van der Giesen 2008) and 30% (International Energy Agency 2011) respectively. An overview of the relevant details for the modelled power plants with and without carbon capture and compression to 25 bars can be found in the supplementary information.

Direct air capture (DAC)

Capturing CO₂ from the atmosphere, also called direct air capture (DAC), is an industrial technology already used for decades in air revitalization systems on submarines and in space vehicles (Herzog 2003) and is considered as a future option for reducing global atmospheric CO₂ concentrations (Olah et al. 2011; Keith 2009; Zenz House et al. 2011). Until now, there has been no experience with large scale application of the technology (Keith 2009) ,and thus solid and transparent information of air capture technology used on larger scales is limited (Herzog 2003; Zenz House et al. 2011). Two routes are proposed for air capture (Stechel and Miller 2013; Olah et al. 2011). One route is using basic absorbents like calcium-, potassium or sodium hydroxides to bind the CO₂ from the atmosphere and regenerate the formed carbonates to release the CO₂ again. Because of the extreme high energy demands related to the regeneration of these absorbents, recent developments focus on the second and less energy intensive route. This route is based on the moisture swing process as developed by Klaus Lackner (2009). This process uses anionic resins that absorb CO₂ when dry and release it when exposed to moisture. It is demonstrated that simply exposing the resin to water (vapour) would release CO₂ from the resin and that a water temperature of 45°C is sufficient to drive most of the CO₂ off the resin and have it revert to the carbonate state that it can be re-used. The sorbent can be regenerated many times without degrading (Lackner 2009). For now we assume that the resin can be used infinitely and that life cycle environmental impacts are so low, that modelling of the resins is not necessary. Lackner proposes a CO₂ capture device that consists of a wind driven filter system, covered with resin, through which ambient air is led and a CO₂ compressor (67 bar) contained in a cargo container (12 m x 2,5m x 3 m). One of these units should be able to collect 1 ton of CO₂ per day. Additionally all the heat that is needed will be produced as an incidental by-product of the compressor. In total 50 kJ / mol CO₂ or 1,1 MJ (=0,31 kWh) electrical energy / kg CO₂ is needed (Lackner 2009).

3.3 Results and impact assessment

Different routes to produce liquid hydrocarbon fuels from CO₂ with existing technologies as defined in Table 1 were assessed on their net greenhouse gas (GHG) emissions and cumulative energy demand (CED) and compared with relevant existing liquid fuel routes. To calculate the net GHG emissions the characterization factors relating to GWP 100 from the CML 2001 impact methodology were used and extensions for biogenic CO₂ and biogenic CO (biogenic addresses emissions from biomass combustion) were added. Also the uptake of CO₂ from the air as a result of biomass growth or using DAC is accounted for. The energy taken into account in calculating the CED is the amount of energy withdrawn from nature (Frischknecht et al. 2007). This is defined as the total energy available in biomass after growth, the energy content of crude oil or the energy that is sent from a PV panel to the inverter. The following paragraphs show the schematic system layouts for this routes and discuss their GHG and CED performance.

Producing synthetic fuels from fossil fuel based CO₂ and energy

The top part of figure 3.2 shows a system in which CO₂ and electricity from natural gas combustion are used to produce liquid synthetic fuels. To produce and combust 1 MJ of synthetic fuel this system emits 0,29 kg of CO₂-eq, of which 0,05 kg are emissions from background processes for example needed to build the required infrastructure. The main GHG emitting process is the generation of additional electricity. To generate and capture sufficient CO₂ to produce 1 MJ of liquid fuel 1,5 MJ of natural gas is combusted. The additional electricity is obtained by combusting another 2,9 MJ of natural gas without capturing the emitted carbon dioxide. Energy needed in background processes is 0,68 MJ. This means that in total 5 MJ of primary energy is required to produce 1 MJ of liquid fuel.

Existing alternatives to producing liquid hydrocarbon fuels from fossil resources are conventional diesel or GTL diesel. Both show an expected better performance than the NGNG route described above but do not start from CO₂ as a feedstock. If we apply ecoinvent data (von der Assen et al. 2013) on conventional diesel production in our LCA model including its combustion, the outcomes show a CED of 1,25 MJ / MJ and emits 0,08 kg CO₂-eq/MJ. A system for GTL diesel shows a CED of 1,7 MJ/MJ and emits 0,11 kg CO₂-eq / MJ.²⁴

The biggest share of the total GHG emissions and CED is connected to the generation of additional electricity. A straightforward improvement can therefore be sought in adjusting this process, for example by using PV electricity to provide the additional electricity. The bottom part of figure 3.2 shows such a system. This system shows an

improved performance over the previous but still performs worse than conventional or GTL diesel. The weak performance of both natural gas-based systems is especially visible in their CED scores. These high scores are mainly caused by the inefficient use of natural gas through combustion in which carbon and hydrogen atoms are separated. It is more efficient to use existing CH bonds, present in fossil fuels, than to combine these atoms artificially.

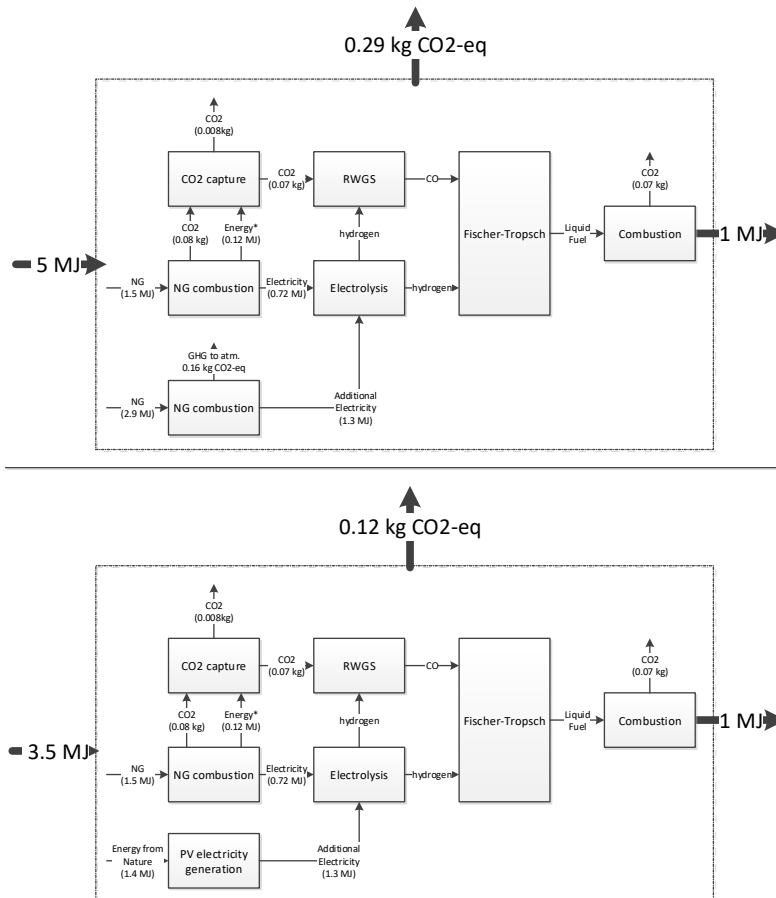


Figure 3.2: Liquid fuel production from natural gas based CO₂ and energy (NGNG) on the top and from natural gas based CO₂ and PV electricity on the bottom (NGPV).

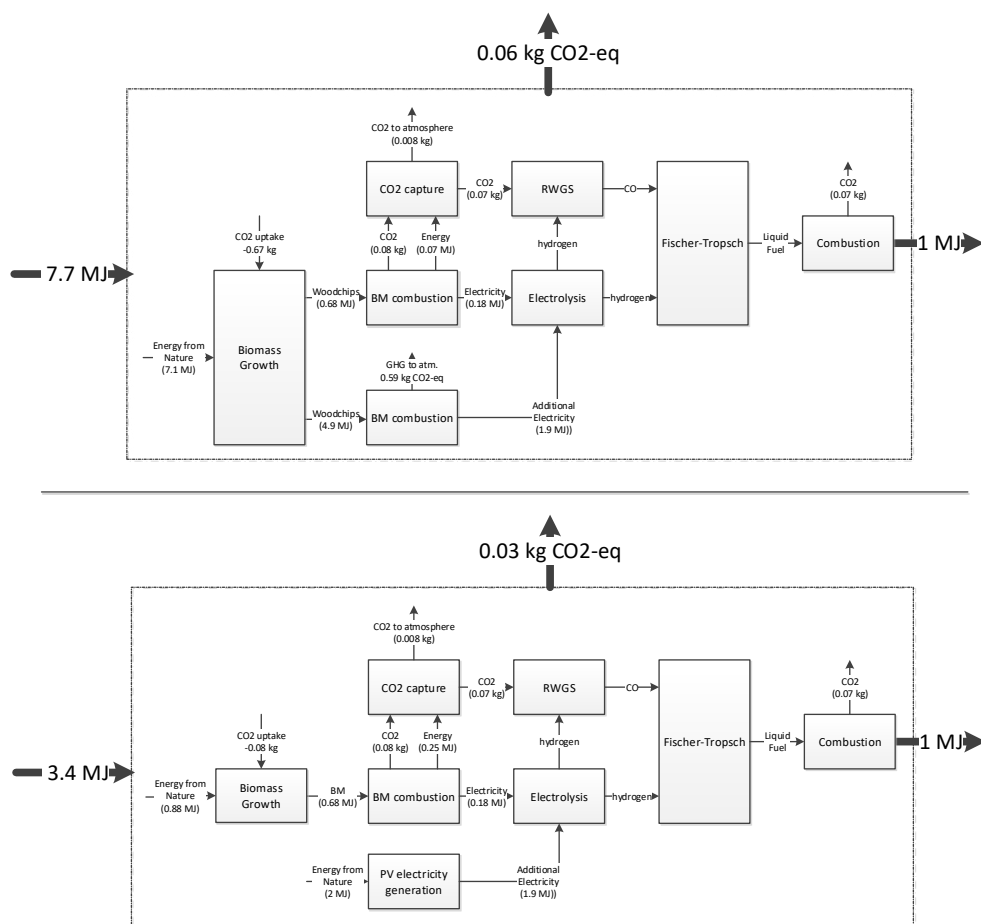


Figure 3.3: Liquid fuel production from biomass based CO₂ and energy (BMBM) on the top and from biomass based CO₂ and PV electricity on the bottom.

Producing synthetic fuels from biomass based CO₂ and energy CO₂ and energy can also be generated through biomass combustion. Because biomass has taken up the CO₂ shortly before it was harvested, the use of CO₂ from biomass combustion is intuitively assumed to be carbon neutral. Figure 3.3 shows a system layout to produce synthetic fuels from CO₂ and electricity from biomass combustion. The production and combustion of 1 MJ of synthetic fuel produced from biomass emits 0,06 kg of CO₂-eq which are all caused by background processes. Also in this system the main GHG emitting process is the generation of additional electricity, while the use of biomass causes a total uptake of 0,67 kg CO₂. To generate sufficient CO₂ and electricity to produce 1 MJ of synthetic liquid fuel, 0,68 MJ of biomass, here in the form of woodchips, needs to be combusted in a power plant equipped with carbon capture technology. For the additional electricity

another 4,9 MJ of woodchips is combusted without carbon capture. To generate this amount of woodchips in total 7,1 MJ of energy was taken up by biomass. In total 7,7 MJ of primary energy is required to produce 1 MJ of liquid fuel from biomass. In comparison with the previously discussed alternatives this system shows lower GHG emissions but much higher energy demand than producing synthetic fuel from natural gas, GTL diesel or conventional diesel. The main cause for this large energy demand is the energy that is lost in converting biomass into woodchips that can be used in a biomass fired power plant and the low efficiencies of biomass combustion.

Existing alternatives to produce liquid hydrocarbon fuels from biomass are ethanol from sugar cane or BTL diesel. Both show an improved performance. By using ecoinvent data in our LCA model it can be derived that ethanol has a CED of 2,9 MJ / MJ and emits 0,04 kg CO₂-eq/MJ. BTL diesel shows a CED of 2,1 MJ/MJ and emits 0.01 kg CO₂-eq/MJ (Elgowainy et al. 2012).

Also for the biomass alternative the largest contributing process to GHG emissions and CED is the generation of additional electricity. The bottom part of Figure 3.3 shows a production system in which the additional electricity produced from biomass is replaced by PV electricity. This system shows a better performance compared to biomass FT fuels but performs worse than BTL diesel and slightly better than bio-ethanol regarding GHG emissions. The CED score is worse than both alternatives which is mainly caused by the inefficient use of biomass through combustion and the energy needed to combine carbon and hydrogen atoms, as in the natural gas route.

Producing synthetic fuels from atmospheric CO₂ and PV electricity

Another source for CO₂ is the atmosphere. The energy needed to capture CO₂ from the atmosphere and to generate the required amount of hydrogen can be obtained from non-carbon energy sources, for example PV electricity. In Figure 3.4 a possible system layout is presented.

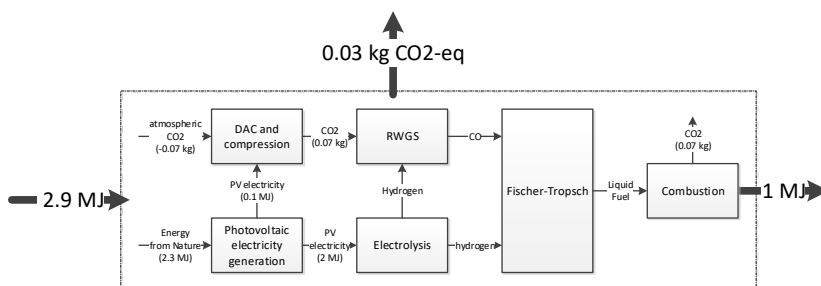


Figure 3.4: Liquid fuel production from atmospheric CO₂ and solar electricity (DACPV).

In total, the system emits 0,03 kg of CO₂-eq if 1 MJ of liquid fuel is produced and combusted. The net GHG emissions are the result of background processes. In total 2,9 MJ of energy is taken up from nature of which 2,3 MJ is transferred into electricity to capture CO₂ and mainly generate hydrogen. The remaining 0,6 MJ is taken up by background processes. Producing synthetic fuels through this system shows an improvement over existing liquid hydrocarbon fuels, like diesel and ethanol, production systems regarding total GHG emissions. This alternative has the best CED performance of all routes producing synthetic fuels from CO₂, but is still worse than existing fuel routes.

Figure 3.5 and figure 3.6 give an overview of the impact assessment results. In these figures, one extra alternative is added, being solar hydrogen. This alternative does not concern a hydrocarbon fuel, but is expected to be one of the promising transportation fuels in the shorter run, a possible energy storage medium and an intermediate product for producing hydrocarbon fuels from CO₂. It is therefore considered as an important competitor in fulfilling the claims presented in the introduction of this study. Although attention needs to be given to the fact that the required hydrogen infrastructure is not considered here. Solar hydrogen can be produced through water electrolysis with PV electricity and is compressed to around 300 bars to be used in existing hydrogen buses (Rovers 2005). Producing and using 1 MJ hydrogen at a pressure of 300 bars emits 0,02 kg CO₂-eq emissions and uses 2,3 MJ of energy.

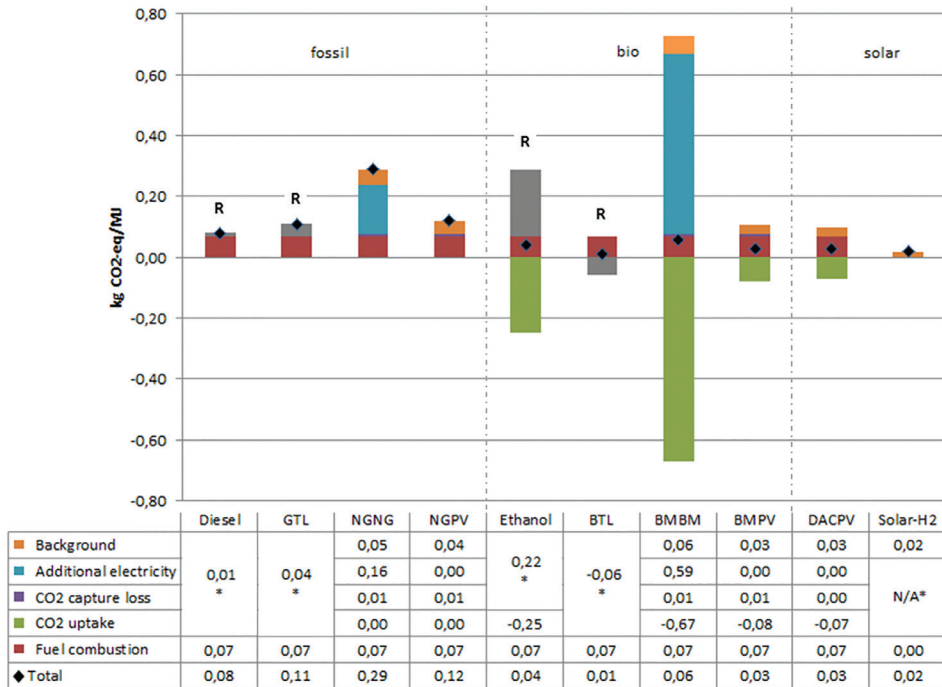


Figure 3.5: GHG emissions of different liquid fuel production routes related to a functional unit of 1 MJ. (*The data for diesel, GTL, ethanol, BTL and solar hydrogen cannot be divided into the uptake of CO₂ and connected processes and are therefore aggregated. R indicates reference alternatives not explicitly modelled in this study.)

In Figure 3.5 the GHG emissions for all alternatives discussed are displayed. It is clearly displayed that fossil based production of synthetic fuels does not show any improvement over existing liquid hydrocarbon production routes based on fossil fuels. Considering bio-based fuel production routes, large quantities of carbon dioxide are taken up from the atmosphere, the related background emissions however show that synthetic fuel production is competitive but not a clear improvement in comparison with existing bio fuel routes. Producing liquid hydrocarbon fuels, completely based on solar energy show a competitive result to existing fuels, when looking at GHG emissions.

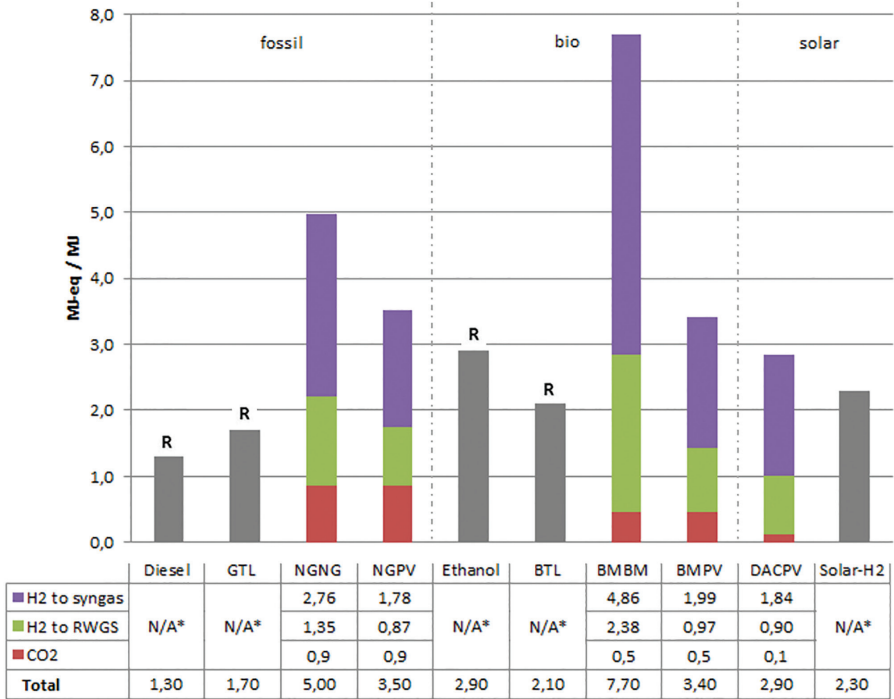


Figure 3.6: Disaggregated CED scores of different liquid fuel production routes related to a functional unit of 1 MJ. (*CED data for diesel, GTL, ethanol, BTL and solar hydrogen are presented in aggregated form since separate production steps for hydrogen and CO₂ cannot be discerned. R indicates reference alternatives not explicitly modelled in this study.)

Figure 3.6 shows an overview of the CED scores for all alternatives. The NGNG and BMBM routes are the least efficient and all synthetic fuel alternatives have higher energy demand than the reference fuel routes. Most energy is not used for producing CO₂ but for providing sufficient hydrogen for both converting CO₂ into CO by RWGS and for producing the syngas that is converted into FT fuel.

The CED scores can also be divided into the use of renewable and non-renewable energy sources (Figure 3.7). The synthetic fuel systems described here all use more energy than existing hydrocarbon fuels, but this energy is for a large part renewable energy and therefore often regarded as freely available.

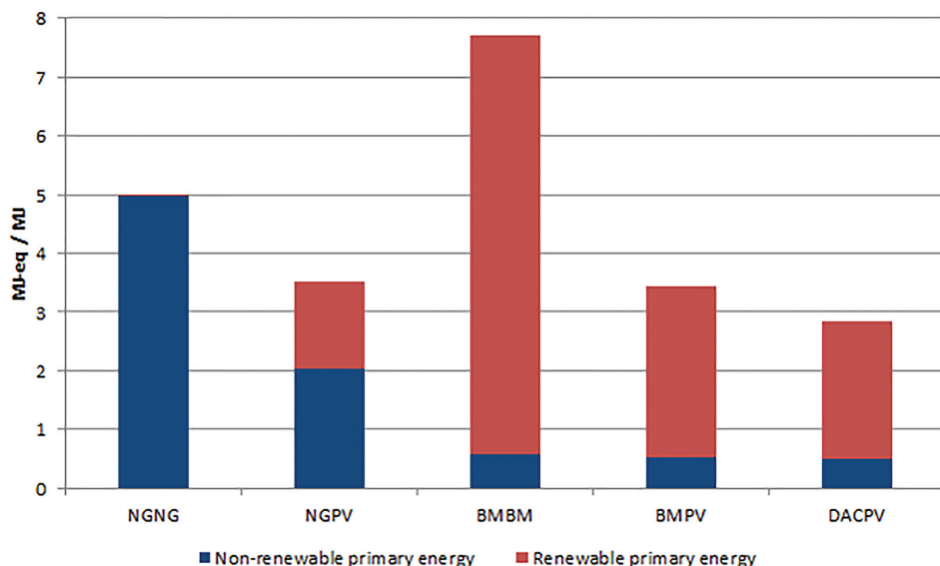


Figure 3.7: Contribution of non-renewable and renewable energy to cumulative energy demand related to a functional unit of 1 MJ.

3.4 Discussion

Synthetic liquid hydrocarbon fuels produced from CO_2 and solar energy have been proposed to contribute to a sustainable energy future. In this study we have investigated four arguments in favour of this claim from the recent public and scientific discourse. Our analysis is based on peer-reviewed data and the results should however be regarded as a first attempt to quantify the CO_2 emissions and energy demand of fuel production from CO_2 . This is certainly the case for the DAC technology because this technology is still in the early stages of development and data for industrial scale operations is still lacking.

The claim that fuels produced from CO_2 are renewable is countered. It is shown that even the best performing fuel production route, which is DACPV, both now and in the near future depends on non-renewable fuels and large amounts of renewable electricity. Where the non-renewable energy demand comes from background processes, it can be argued that renewable energy can be deployed for reducing atmospheric CO_2 concentrations more efficiently by replacing fossil based electricity directly than by producing fuels from CO_2 (Graves et al. 2011).

Second, it was claimed that carbon neutral fuels can be produced when overabundant CO_2 is used. The present study clearly shows that using CO_2 from a fossil origin will

not provide a carbon neutral fuel. This supports an earlier claim by Dumont (2012) that “positive environmental effects of a CO₂ consuming reaction cannot be taken for granted” (Dumont et al. 2012). Using atmospheric CO₂ is the best option but does not provide a carbon neutral fuel because of the CO₂ emissions related to fossil energy demand in background processes. This implies that carbon neutral fuels might be produced from CO₂, but only in a future energy system completely based on renewable energy.

The third claim, that producing fuels from CO₂ presents a route to storing renewable energy cannot be completely supported or countered from the LCA results presented here. It is clear that producing fuels from CO₂ by using solar electricity converts solar energy into chemical - and therefore easy to store - energy. To assess if this is a preferable route to store energy, additional research is needed in which the production and use of fuels from CO₂ needs to be compared with battery and hydrogen storage and possibly others storage options, such as water reservoirs.

The fourth argument, that fuel production from CO₂ is preferable to CO₂ sequestration has already partly been countered in the introduction by explaining that producing a fuel from CO₂ neglects the primary goal of carbon sequestration. This counter argument is further supported by the fact that far more energy is needed to produce a fuel from CO₂ than it will deliver when combusted. It would be far more profitable to sell the required energy directly on the market than to lose a great deal of energy in the inefficient production of liquid fuels.

In conclusion, we state that the energy demand and climate impacts of using CO₂ to produce synthetic hydrocarbon fuels by using existing technologies are higher than the impacts of existing hydrocarbon fuels. The intuitive claims in the public discourse cannot be supported by our quantitative assessment which shows that producing liquid fuels from CO₂ is not the straightforward panacea as suggested. However, novel technologies (e.g. photocatalytic, solar thermal and enzyme based routes) might show a slightly improved system performance.

In a distant future, we foresee possible niches for hydro carbon fuels produced from CO₂. Since hydrocarbon fuels offer high energy to mass and volume ratios compared to alternatives like electricity and hydrogen, the application of fuels produced from CO₂ in applications such as airplanes and heavy duty transport may prove to be a valuable but future niche. Another application could be as a storage medium for so-called stranded renewables. Because renewable energy technologies produce difficult-to-store electricity and renewable electricity supply increasingly exceeds demand, research has begun in

levelling supply and demand using concepts such as smart grids. Even in smart grid systems it can be expected that some sort of energy storage will still be needed. For storing large amounts of renewable energy, the production of synthetic hydrocarbon fuels is one of the technologies that could be used. However, it would have to compete with other storage technologies such as batteries, hydrogen storage, water reservoirs or compressed air storage.

Acknowledgements

This project was carried out within the research programme of Bio Solar Cells, co-financed by the Dutch Ministry of Economic Affairs, Agriculture and Innovation.

3.5 Appendix

This appendix contains the supporting information for this case study and includes details on the modelled processes, supporting calculations.

3.5.1. Foreground process descriptions

Hydrogen generation and supply

Hydrogen is mostly produced from natural gas and, because of its fossil origin, cannot be considered as sustainable or renewable energy carrier. Therefore it needs to be produced by using solar energy as the energy source. According to Tributsch (2008): “the simplest and most elegant photovoltaic hydrogen generator consists of a solar cell and an electrochemical device, an electrolyser, which is liberating hydrogen from liquid water.” From the different routes to electrolyze water the process which uses an alkaline electrolyte is the most evolved and widely used (Tributsch 2008) and will therefore be the process used in this exercise. Typically this electrolyte is potassium hydroxide (KOH) that is supplied via a 25 -30% aqueous solution (Kruse et al. 2002; Pagliaro, M. Konstandopoulos et al. 2010; Ivy 2004) and which can be retrieved and reused in the process (Pagliaro, M. Konstandopoulos et al. 2010). Here we consider the production of hydrogen via water electrolysis using photovoltaic (PV) electricity.

Background data for modelling the process of hydrogen production by electrolysis is taken from work performed by Rovers (2005) and Sumner (2006). Both have modelled the production of hydrogen by electrolysis. An overview of the foreground processes modelled in this study can be found in figure 3.8.

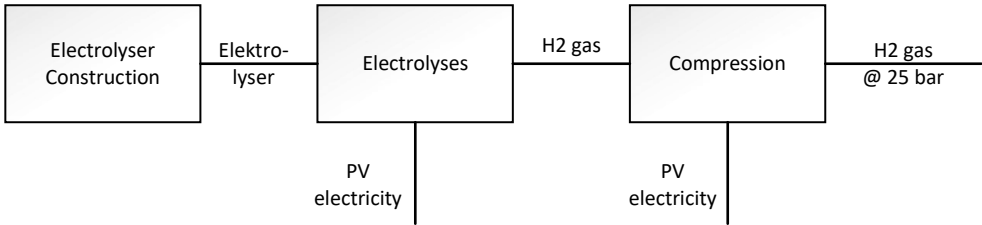


Figure 3.8: LCA scheme: Electrolysis of water for hydrogen production (foreground processes).

Electrolyser construction

Data for the Electrolyser (60 m² Hydrogen / hour) is based on Rovers (2005) in which background data from Ecoinvent 1.01 is used. To use this data with the Ecoinvent 2.2 database (Swiss Centre for Life Cycle Inventories 2010) a number of processes have been adjusted. First Rovers used an input of sodium hydroxide which has been changed to potassium hydroxide (KOH). Second, Rovers states that for purging the Electrolyser during maintenance, nitrogen and hydrogen are used and emitted. The updated process contains this amounts of nitrogen as well, the hydrogen can be considered as product emitted to the atmosphere (product loss) resulting from venting the system and is not modelled as an economic input but as an emission. In Table 3.2 all adjustments executed are stated.

Table 3.2: Electrolyser construction, updated from Rovers (2005).

Rovers (2005)	Rovers (2005), updated to Ecoinvent 2.2 data
Economic inputs	Economic inputs
Sodium Hydroxide, 50% in H ₂ O, production mix, at plant, (RER)	Potassium hydroxide, at regional storage (RER)
Transport, lorry 32 t (RER)	Transport, lorry 16 -32t, EURO 3 (RER)
	Added: Nitrogen, liquid at plant (RER)
<i>Resources</i>	<i>Resources</i>
Occupation, industrial area, built up (landscape)	Occupation, industrial area, built up (resource_land)
<i>Emissions</i>	<i>Emissions</i>
Nitrogen	Cut-off; no environmental impact is associated with nitrogen to air.
Hydrogen	Hydrogen (air_unspecified)

Electrolysis

Data for the electrolysis process itself is based on the process modelled by Sumner (Sumner 2006) and uses the electrolyser modelled above. Sumner's process is compared with existing research and publications on electrolysis (see Table 3.3) which shows no large variety among different data sources.

Table 3.3: Overview of literature on electrolysis; economic inputs per kg hydrogen (STP).

Reference	Inflows		Additional information
	Water	Energy	
Kruse et al. (2002)	N/A	50,1 kWh	$\eta_{\text{sys}} = 80\%$
Pagliari et al. (2010)	N/A	44,5 – 54,5 kWh	$\eta_{\text{sys}} = 55 - 75\%$, 25-30% KOH aq. solution
Ivy (2004)	11.1 kg	46,7-48,7 kWh	$\eta_{\text{sys}} = 80\%$
Sumner (2006)	11.1 kg	56,7 kWh	N/A
Levene et al. (2006)	N/A	39 kWh	1 bar / 25°C
Stojic et al. (2003)	N/A	50,1 – 55,6 kWh	-
IEA (2007)	N/A	48-60 kWh	1 – 25 bar / 70-90°C
NEL Hydrogen (2012)	10 kg	45,6-48,3 kWh	1 bar / 80 °C, $\eta_{\text{sys}} = 80\%$, 25% KOH aq. sol.
Hydrogenics (2012)	16,7 -22,2 kg	54,5-60,1kWh	1 bar / 80 °C, 30% KOH aq. Solution, HySTAT electrolyser

*Values in this table are all recalculated to the production of 1 kg hydrogen, 1 kg of hydrogen outflow is considered as 11,1 Nm³.

Assuming a lifetime of 10 years an 8000 hours operation a year, one needs $2,31 \times 10^{-6}$ electrolyzers to produce 1 kg of hydrogen gas. Table 3.15 shows the economic inputs for the production of 1 kg of hydrogen gas.

Hydrogen compression

Hydrogen is produced at atmospheric pressure and temperature. For the other processes downstream in the FT fuel production chain, the hydrogen needs to be pressurized to 25 bar. For compressing hydrogen the process in this study is modelled by using information from Sumner (2006). Sumner modelled a compressor that compresses hydrogen to 85 bars, requiring 2,23 kWh / kg hydrogen. Because the present study assumes a pressure of 25 bars the energy requirements for compression are $25 / 85 * 2,23 = 0,66$ kWh/kg.

Assuming a compressing capacity of 300m³/hr, a 10 year lifetime and 8000 hours operation a year one needs $3,42 \times 10^{-8}$ compressor to compress 1 kg hydrogen gas. In

Table 3.16 and Table 3.17 the economic inputs for compressing 1 kg of hydrogen to 25 bar can be found.

Syngas production via RWGS

Haije and Geerlings (2011) suggest to use the reverse water-gas shift reaction (RWGS) to produce carbon monoxide (CO) that will be blended with hydrogen to form syngas (see Figure 3.9). The data used in modelling this process is checked with the authors via personal communication.

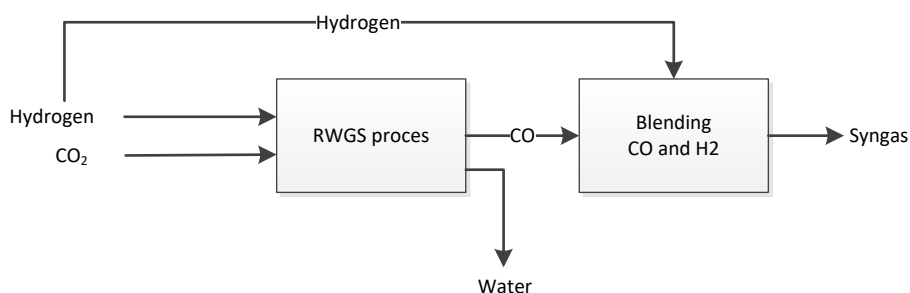


Figure 3.9: General overview of syngas production.

The RWGS reaction is an endothermic equilibrium reaction. At lower temperatures the conversion of CO₂ and H₂ into CO is 100% stoichiometric, regarding that all water that is produced in the reaction is selectively removed to prevent the back reaction, called water gas shift (Haije and Geerlings 2011). With a simple lab experiment it is shown that CO can be produced from CO₂ and H₂ in a fixed bed reactor which contains a mixture of a WGS catalyst and a water sorbent. The heat that is released by the sorbent reaction inside the reactor is considered to be sufficient to drive the RWGS reaction. Excess heat from the Fischer-Tropsch reaction downstream in the FT fuel production process can be used to regenerate the sorbent (Haije 2013). It is assumed that after a 30 minute cycle of CO generation another 30 minute cycle of sorbent regeneration is required per reactor. Using two reactors at the same time, one in adsorbing and the other in desorbing modus, makes a continuous process possible (see Figure 3.10).

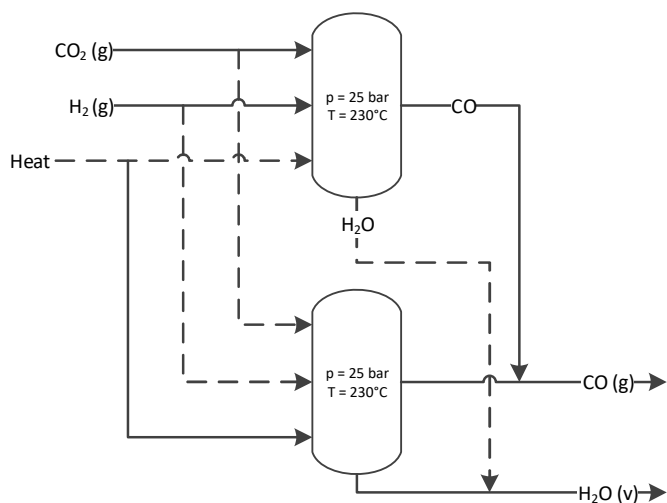


Figure 3.10: Hypothetical configuration RWGS process using two reactors.

For modelling the RWGS process in an LCA model the foreground processes as shown in Figure 3.11 are considered. In order to produce carbon monoxide via the RWGS process a fixed bed reactor and chemicals like a water sorbent and RWGS catalyst are needed. Below short descriptions of modelling these flows and processes are given.

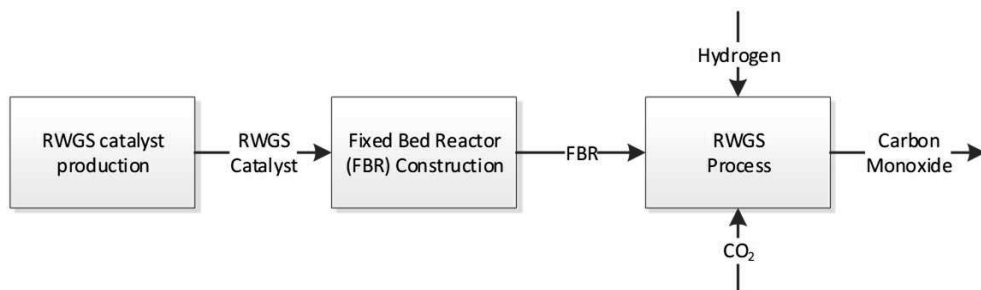


Figure 3.11: Hypothetical configuration RWGS process using two reactors.

RWGS catalyst and water sorbent

As RWGS catalyst Südchemie Shiftmax 240 is proposed. This catalyst consists of 57% CuO, 31% ZnO and 11% Al₂O₃. In the LCA model the RWGS catalyst is assumed to be composed as presented in Table 3.18.

As water sorbent zeolite (Merck) is proposed, which is modelled as zeolite powder provided by the Econinvent v2.2 database. Both chemicals are assumed to be regenerated infinitely and are therefore considered as part of the fixed bed reactor.

Fixed bed reactor construction

The fixed bed reactor is assumed a steel vessel as shown in Figure 3.12.

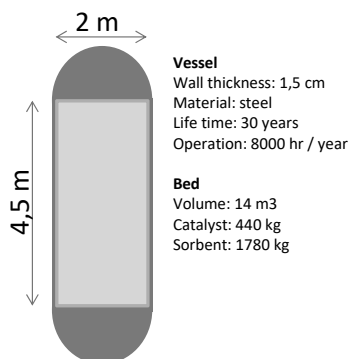


Figure 3.12: Hypothetical fixed bed reactor.

The reactor vessel consists of 4760 kg of steel (assuming 50% low alloyed steel and 50% chromium steel) and is filled with a mixture of 440 kg of RWGS catalyst and 1780 kg of sorbent, which need to be renewed every 4 years (Haije 2013). Over a reactor lifetime of 30 years therefore $30/4 \times 440 \text{ kg} = 3300 \text{ kg}$ of catalyst and $30/4 \times 1780 \text{ kg} = 13350 \text{ kg}$ of sorbent is needed. Since two identical reactors are used in parallel all numbers are doubled in the unit process representing the construction of the fixed bed reactor (see Table 3.19).

RWGS process

With regard to the Fischer-Tropsch (FT) reaction downstream for which the produced carbon monoxide is an inflow it is assumed that the RWGS reaction takes place at a pressure of 25 bars and a temperature of 230°C, being high enough for proper performance of the FT catalyst. It is assumed that the experimental outcomes (retrieved from a 1 bar reactor) can be extrapolated to the conditions above. All flows are related to the production of 1 kg of carbon monoxide gas @ 25bar / 230°C (Haije 2013).

By extrapolating Haije's experimental results, it can be assumed that 2900 kg of CO gas can be produced in one cycle of 30 minutes, or 1 kg CO gas / 0,6 seconds. Considering a reactor lifetime of 30 years and 8000 operating hours a year, the production of 1 kg of CO gas requires the input of $1,93 \times 10^{-9}$ fixed bed reactor.

For every kg of CO produced also 0,64 kg of water vapour is produced as a by-product. In this study this flow is not modelled (cut-off), but it can be considered to use this flow as a (partial) water input for other processes. Table 3.21 shows the in- and outflows of the RWGS process in this study.

Producing syngas by blending carbon monoxide and hydrogen

For obtaining syngas with the required $H_2 : CO$ ratio of 2 : 1, hydrogen and carbon monoxide gas are blended. The syngas has a calculated net heating value of 23,9 MJ/kg and a calculated density of 0,470 kg/m³ (@ 273 K / 1 bar) or 6,38 kg/m³ (@ 503K / 25 bar). Producing 1 kg of syngas requires blending 0,125 kg hydrogen with 0,875 kg carbon monoxide.

Gas to liquids conversion (GTL)

For modelling the GTL process in the present study general numbers from public literature combined with public available data on the Pearl GTL plant in Qatar, operated by Shell are used and checked with Shell GTL specialists. In general producing liquid fuels from gas takes place as presented in Figure 3.13. First natural gas is transferred into syngas and liquefied natural gas products like LPG, Ethane and condensate. The syngas is then fed into the Fischer-Tropsch (FT) reactor where it is converted into syncrude that is subsequently cracked into a variety of GTL products like Naphta, Kerosene, Gasoil and Base-oil. In the Shell's Pearl GTL facility in Qatar daily 120.000 barrels of gas products are produced and 140.000 barrels of GTL products.

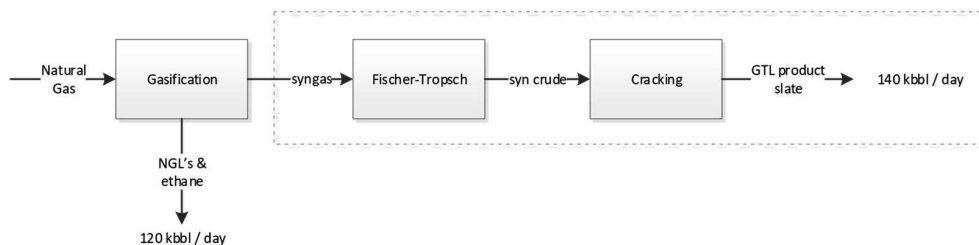


Figure 3.13: General GTL process lay-out.

For this study we will focus on the processes within the dotted line in Figure S6. The syngas used in the FT-process has a hydrogen : carbon monoxide ratio of 2 : 1 (Eilers et al. 1990; Reinalda 2013). The FT process takes place in a fixed bed reactor in which it is run over a metal based catalyst, in this study cobalt is assumed as being the main component, where the syngas is converted to syncrude. The FT process is an exothermic reaction, which takes place at pressures between 20 – 60 bars and temperatures 180 – 250°C (Tijmensen et al. 2002; Boerigter et al. 2004). Here we assume the FT reaction to take place at 25 bars and 230°C. FT efficiencies have been reported from 70% (Tijmensen et al. 2002) to 80% (Boerigter et al. 2004; Forman et al. 2011), meaning that 80% of the energy available in the syngas is transferred into syncrude. The remaining 20% consists of hydrocarbon chains that are too short to convert into fuels and which are mainly used to generate electricity to run the GTL plant and of heat that can be used

to produce steam. In this study it is assumed that the energy not transferred into fuels is completely used for internal energy and for regeneration of the RWGS catalyst and is not modelled separately. The efficiency for the hydrocracking process in which syncrude is transferred into different GTL products is assumed as 100% (Boerigter et al. 2004). The GTL process that will be modelled here, has a syngas to GTL product efficiency of $1 \times 0,8 = 80\%$ (see Figure 3.14).

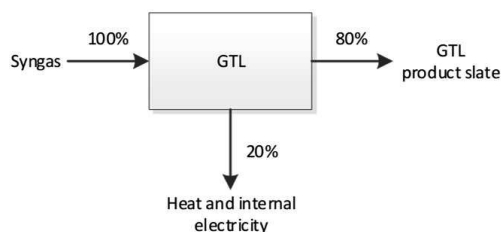


Figure 3.14: General energy balance GTL process.

The Pearl GTL plant in Qatar is designed for optimal diesel production. The GTL products are divided into naphtha, kerosene, gasoil and base oil (Gainsborough 2009). Using the efficiencies discussed above and this product slate the quantity of syngas required is calculated on the basis of energy content, using the syngas properties calculated before (see Table 3.4 for details). The FT fuel regarded in this study that is produced is a mix of all products produced. Its LHV value is also derived from the same table and is set at 43,2 MJ/kg.

Table 3.4: GTL in- and outflows energy balance.

	Density	Production			Net caloric value	Energy content	Energy content
Products OUT	[kg/m ³]	[kbbbl/day]	[m ³ /day]	[ton/day]	[MJ/kg]	[GJ]	[%]
Naphtha	768	35	5.565	4.274	44,5	190.189	19%
Kerosene	800	25	3.975	3.180	45,0	143.100	15%
Gasoil	832	50	7.950	6.614	43,3	286.404	29%
Base oil	860	30	4.770	4.102	40,2	164.908	17%
Total Product slate		140	22.260	18.171	43,2	784.601	80%
Heat	N/A	N/A	N/A	N/A	N/A	196.150	20%
Product IN							
Syngas	6,38	N/A	N/A	40.967	23,94	980.752	100%

*kbbbl = 1000 barrel = 1000 x 159 litre.

Based on the Shell GTL process as presented above a LCA unit process is constructed in Figure 3.16.

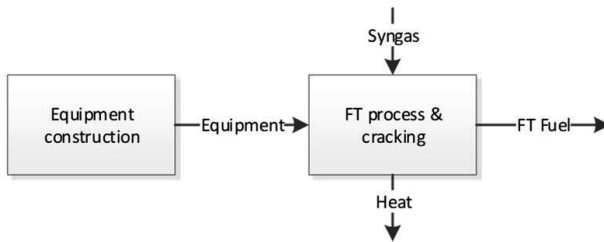


Figure 3.15: LCA unit process for GTL.

GTL Plant

The material demand of the required GTL plant is based on publicly available data and comprises the use of concrete, steel and the area occupied by the plant. An overview of required materials is given in Table 3.5.

Table 3.5: LoremMaterial requirements for GTL plant.

Resource	Value	Reference
Land area	1.4 x 1.6 km = 2.240.000 m ²	Green Car Congress (2006)
Steel use	24 steel reactors weighing 1200 ton each = 28.800 ton	Shell (2009a)
Concrete	690.000 m ³	Shell (2009b)

Since the gasification step is excluded from the process considered here, only about half of the plant materials are required. Resulting of an input of 1.120.000 m² of land, 14.400 ton of steel in an assumed equal division of reinforcing and low alloyed steel, 345.000 m³ of concrete (Table 3.22).

GTL production

Based on energy contents of flows and an assumed GTL plant efficiency 80% the GTL plant converts 2,3 kg of syngas to 1 kg of GTL product with an average heating value of 43,2 MJ / kg. Concerning that the Shell Pearl GTL plant in Qatar has a production capacity of 140.000 barrels or around 18.000 ton (1000 kg) per day. Assuming 300 days operation per year and lifetime of 30 years for the reactor, per kg of solar fuel 1 / (300*30*18000*1000) = 6,7 x 10⁻¹² reactor is needed.

Energy and carbon dioxide supply

To produce 1 kg of synthetic fuel using these technologies 3,16 kg CO₂ and 24,6 kWh of electricity is needed (see Figure 3.20). When we want to convert all CO₂ into solar

fuel a ratio between electricity and CO₂ can be calculated; being 24,6 kWh / 3.16 kg CO₂ = 7,78 kWh / kg CO₂.

We assume that electricity and CO₂ are supplied in a combined manner by combusting natural gas and biomass to generate electricity and capture the emitted CO₂ by post-combustion carbon capture. Electricity and CO₂ can also be generated independently via photovoltaic (PV) electricity and direct air capture (DAC). The combustion of fuels in this study provides us with two products from one process, which calls for allocation. However, because all the electricity and CO₂ produced in this process are completely used in the downstream processes allocation is not needed.

Natural gas and coal combustion with post-combustion carbon capture

An LCA study on the combustion of natural gas and pulverized coal with post-combustion capture has been done by Van der Giesen (2008). Data for the power plants and fuels supply was based on the Ecoinvent database while carbon capture processes were added. Here we assume that the coal fired power plant and carbon capture plant can be used for the combustion of biomass as well. The power plants used in this study are based in Spain.

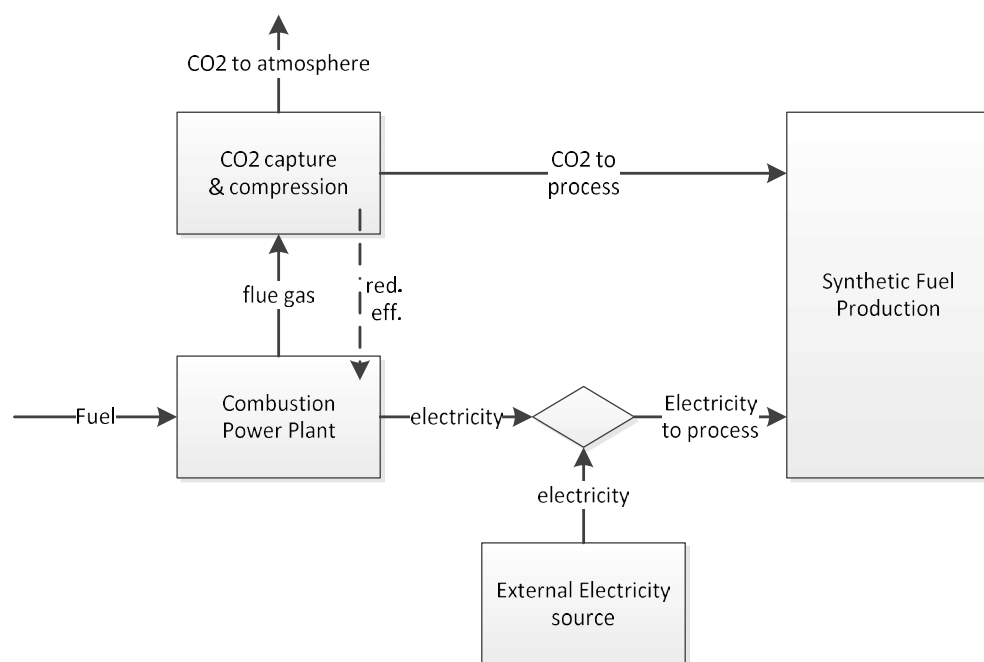


Figure 3.16: Fuel combustion with post combustion carbon capture for electricity and CO₂ generation.

When equipped with carbon capture the energy output from power plants decreases as a result from energy needed for the carbon capture like pumps and compressing the CO₂ to a pressure at which it can be transferred. The energy penalties are dealt with by decreasing the output of energy produced by the power plants while using the same quantity of fuel input (and related CO₂ emissions). The energy penalties for natural gas and biomass in this study are set at 15% (Van der Giesen 2008) and 30% (International Energy Agency 2011) respectively.

An overview of the relevant details for the modelled power plants with and without carbon capture and compression can be found in the table below. The main article excludes the use of coal because this alternative is worse than using natural gas and the exercise does not provide additional insights.

Table 3.6: Power plant properties.

	NGCC power plant	BM power plant	Unit
Power	400	400	MWe
Efficiency	57,70%	29,70%	%
Lifetime	180000	150000	hours
Operation	8000	8000	hours / year
Annual electricity production	3,20E+06	3,20E+06	MWh
Plant CO ₂ emissions	0,35	1,14	kg CO ₂ / kWh
Annual CO ₂ emission	1,12	3,65	MT CO ₂ / year
CO₂ capture data			
Energy penalty	15%	30%	%
Annual electricity prod, with capture	2,72E+06	2,24E+06	MWh
Annual CO ₂ production (90%)	1,01	3,29	MT CO ₂ / year
Annual CO ₂ emissions to atmosphere	0,11	0,37	MT CO ₂ / year
Synthetic fuel production requirements			
Electricity required per kg CO ₂ for SF prod	7,78	7,78	kWh / kg CO ₂
Electricity available per kg CO ₂ ATP	2,70 (35%)	0,68 (9%)	kWh / kg CO ₂
Additional electricity needed	5,08 (65%)	7,10 (91%)	kWh / kg CO ₂

Biomass combustion and post-combustion carbon capture

For electricity generation by the combustion of wood with carbon capture to supply solar fuel production with energy and CO₂ a hypothetical power plant that uses 100% biomass (short rotation wood) is modelled. The power plant and CO₂ capture plant are assumed to be copies of the pulverized coal fired power plant and capture unit modelled by Van der Giesen (2008). Where this system might not be explicitly representative for a real world situation, it is expected to give valuable insights. Next to that the model is built in such a way that any adjustments that might need to be done in the future are easily implemented. Although the best proven technology for conversion from biomass into energy is combustion of wood, this is mainly done in small and medium sized units. For large scale power plants biomass is co-fired with coal because of limited regional biomass availability. As an overall electrical efficiency of bio electricity 30% is assumed (Nussbaumer 2003). The following paragraphs will explain the explicit modelling choices, assumptions and data sources for modelling biomass combustion with carbon capture, following Figure 3.17.

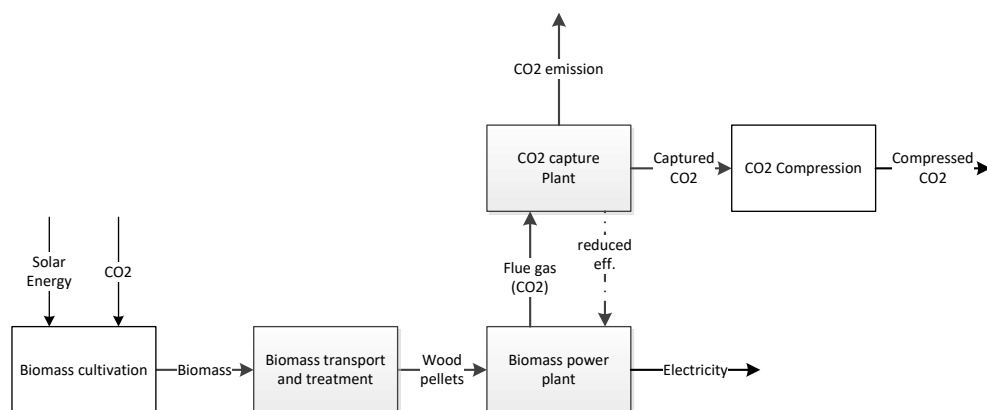


Figure 3.17: Electricity from biomass combustion with post-combustion carbon capture.

CO₂ uptake in biomass cultivation

Data for biomass cultivation are taken from Jungbluth (2008). Jungbluth's data also introduces values for land use and additional environmental extractions and emissions. The most important data provided by Jungbluth are the uptake of 1,78 kg CO₂ and 18,8 MJ of energy per kg of biomass (short rotation wood). These numbers are comparable to the values provided by Sannigrahi (2010).

Biomass treatment

It is assumed that the short rotation wood is converted into wood chips and is transported further to the power plant. This process is directly taken from the Ecoinvent 2.2 database.

for which only the input of wood is changed into short rotation wood as described above. It is assumed that the wood pellets have an energy content of around 18,8 MJ / kg (Jungbluth et al. 2008). Next to that it is assumed that the biomass is taken from a radius of 500 km, transported over 250 km by rail and 250 km by lorry.

Wood pellet combustion and electricity generation

To liberate the energy and CO₂ that has been fixated by biomass (18,8 MJ / kg) it is combusted in a conventional biomass boiler with an efficiency of 78% which produces steam. The steam is subsequently used to generate electricity in steam turbine with an efficiency of 38%. The overall efficiency is therefore 29,6%. It is assumed that the electricity generation can be done in a conventional hard coal power plant as provided in the Ecoinvent database.

The combustion of 1 kg biomass delivers $0,78 \times 18,8 \text{ MJ} = 14,7 \text{ MJ}$ of heat and emits 1,78 kg CO₂. To generate 1 MJ of heat we can calculate that $1 / 14,7 = 0,068 \text{ kg}$ wood pellets are needed which emit $0,068 \times 1,78 = 0,121 \text{ kg CO}_2 / \text{MJ}$.

Producing electricity from this heat with an efficiency of 38% shows that for the production of 1 kWh requires an input of 9,47 MJ of heat. Resulting in plant CO₂ emissions of $9,47 \times 0,121 \text{ kg} = 1,14 \text{ kg CO}_2 / \text{kWh}$ electricity (without carbon capture).

Electricity generation from biomass with carbon dioxide capture

The flue gases containing CO₂ are guided to a post-combustion capture plant using MEA. This system captures 90% of the CO₂ in the flue gases, so that 10% is still emitted to the atmosphere. The capture plant uses energy generated in the power plant which results in a decreased power (electricity) output of 30% (International Energy Agency 2011). This is modelled as follows; a BM power plant without carbon capture uses 9,47 MJ of heat to generate 1 kWh of electricity and emits 1,14 kg CO₂. Connecting a CO₂ capture plant captures 90% of all CO₂ emissions; being $0,9 \times 1,14 = 1,03 \text{ kg}$ decreases the output of electricity to 0,7 kWh. So where 9,47 MJ generates 1 kWh now $9,47 / 0,7 = 13,53 \text{ MJ}$ is required to generate 1 kWh of electricity.

Another important number is the combined generation of 0,7 kWh of electricity and the capture of 1,03 kg CO₂. This means that per kg CO₂, $0,7 / 1,03 = 0,68 \text{ kWh}$ electricity is produced. The process data are copied from the carbon capture process connected to a 400 MW coal fired power plant, as modelled by Van der Giesen (2008). The exact size and resources needed for the process depend on the flue gas flow and composition, which for now is assumed to be comparable for burning coal or biomass.

Additional electricity requirements for SF production

As can be expected and seen in Table 3.7 (and in Figure 3.21) the electricity generated by the combustion power plants is not sufficient to convert all captured CO₂ into solar fuels and additional electricity is needed. This modelled by producing and electricity mix existing of electricity produced by the power plants which is supplemented by grid electricity or PV electricity via the ratios in the table below.

Table 3.7: Electricity mix compositions.

	Power plant	Additional	Electricity mix
NG mix	0,35 kWh	0,65 kWh	1 kWh
BM mix	0,09 kWh	0,91 kWh	1 kWh

Direct air capture (DAC)

Capturing CO₂ from the atmosphere, also named (direct) air capture (DAC), is an industrial technology already in use for decades in air revitalization systems on submarines and in space vehicles (Herzog 2003). Air capture is one of the considered options for reducing global atmospheric CO₂ concentrations as a route to manage global warming (Keith 2009; Jones 2011; Olah et al. 2011). While large scale application of the technology is still not feasible there is a variety of proposed routes for air capture (Olah et al. 2011; Goeppert et al. 2012). The best known and common way is by using basic absorbents like calcium-, potassium or sodium hydroxides to bind the CO₂ from the atmosphere and regenerate the formed carbonates to release the CO₂ again. Another option is to replace the hydroxides by carbonates. These bind more weakly to CO₂ making regeneration easier and less energy intensive. Absorption rates are however slower, requiring more time and a higher amount of sorbents to capture the same amount of CO₂ as achieved with hydroxides (Olah et al. 2011). More recent developments focus on using anionic resins that absorb CO₂ from the air when dry and releasing it when exposed to moisture (Lackner 2009). The latter is the least energy intensive and is therefore taken in the present study.

Restrictions for using NaOH CO₂ capture systems concern costs and energy demand. Lackner (2009) identified more reasons why the NaOH might not be the preferred technology to capture CO₂ from the air. Large binding energies between CO₂ and the sorbent requires high energy demands for regeneration, considerable energy demand is connected to moving the solvent around to prevent it from drying and serious concerns exist over the corrosiveness of NaOH solutions. His research shifted towards the use of a solid strong base ion-exchange resin. By using this resin CO₂ from a gas stream even more dilute than in ambient air can be captured and the required energy is far lower than needed in a process using NaOH (Lackner 2009).

Lackner (2009) proposes a specific approach based on a solid sorbent in the form of an anionic exchange resin, that absorbs carbon dioxide when dry and releases it when exposed to moisture, which is known as moisture swing. Lackner demonstrated that simply exposing the resin to water (vapour) would release CO_2 from the resin and that a water temperature of 45°C is sufficient to drive most of the CO_2 off the resin and have it revert to the carbonate state to be used again. Since the resin only comes in contact with water vapour and not the liquid water source, it is possible to use a salt brine as the source of water. The sorbent, which is comparable to Marathon A resin, produced by Dow Chemicals can be regenerated many times without degrading. For now we assume that the resin can be used infinitely and that life cycle impacts are so low, that modelling is not necessary (Lackner 2009).

Lackner (2009) also proposes a collector design. A CO_2 capture device, consisting of wind driven filter system, covered with resin, through which ambient air is led and a CO_2 compressor (to 67 bar) contained in a cargo container (12 m x 2,5m x 3 m) can collect 1 ton of CO_2 per day. Additionally all heat that is needed will be produced as an incidental by-product of the compression. In total 50 kJ / mol CO_2 or 1,1 MJ electrical energy / kg CO_2 is needed (1,1 MJ electrical energy = 0,31 kWh).³⁴

When modelling this process in our LCA model we assume the collector itself to consist of steel for the container alone and that additional materials are not needed. The resin is not modelled since it is assumed that it can be used infinitely and will therefore have a very limited impact over the lifecycle of the collector. The air capture process itself only requires the collector and a certain amount of electricity. Water use is neglected since water quality is not an issue as described above.

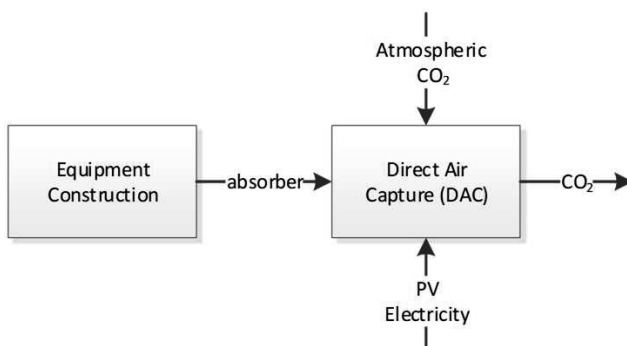


Figure 3.18: LCA unit process for direct air capture (DAC).

The energy supply is modelled in two ways. First the electricity is supplied via CSP, like also done for the NaOH DAC process. Second it is supplied via PV, which seems more logic, and is more efficient, since only electricity (and no heat) is required.

FT fuel combustion

In order to analyse the energy and carbon balances of solar fuel production it is assumed that the solar fuels produced are hypothetically combusted at the gate of the production plant. The outcomes will show how much energy is consumed to produce 1 MJ FT fuel and how many GHG emissions are emitted. The table below provides the relevant fuel properties and assumptions that are used for calculation in this study. For CO₂ emissions theoretical values are calculated based on stoichiometric chemical formulas for combustion. The LHV for FT fuels is an average value calculated from of the LHV values of the possible GTL product slate (Table 3.4).

Table 3.8: Selected (alternative) fuel properties.

Fuel	Formula	CO ₂ emission from combustion		LHV		density
		kg CO ₂ / kg Fuel	kg CO ₂ / MJ fuel	MJ/kg	kg/MJ	
Diesel	C ₁₃ H ₁₈	3,11	0,0716	43,4	0,0230	751
Ethanol	C ₂ H ₆ O	1,91	0,0714	26,8	0,0373	789
FT Fuel*	C ₁₃ H ₁₈	3,11	0,0716	43,2	0,0231	816

*Data taken from this study, CO₂ emission are assumed to be comparable to fossil diesel

For the GTL alternative that use fossil based energy and CO₂ (NG), the CO₂ emissions are defined as fossil based. For the bio-based alternatives, the CO₂ emissions are defined as biogenic.

Solar Hydrogen production

Figure 3.19 shows the unit process for generating hydrogen through electrolysis with PV electricity.

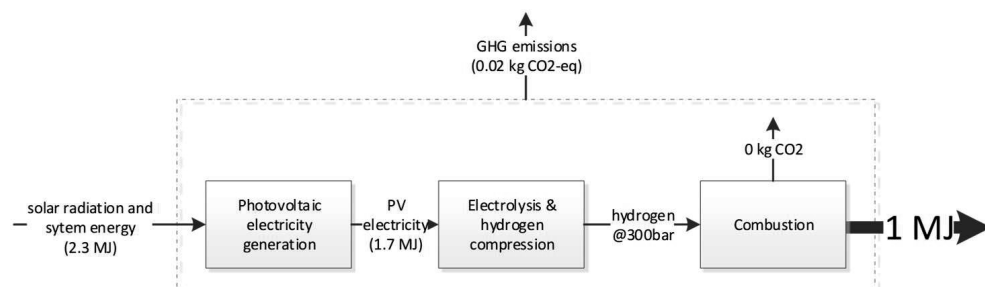


Figure 3.19: LCA unit process for solar hydrogen production and use (including LCA outcomes).

3.5.2. System calculations

Energy and carbon dioxide demand for FT fuel production.

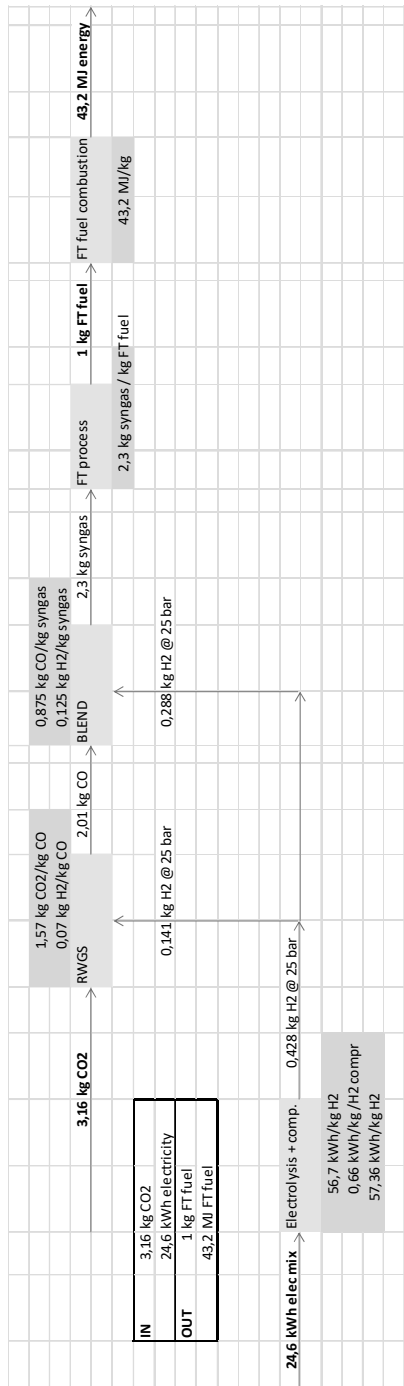


Figure 3.20: Carbon dioxide and electricity demand for FT fuel production.

Electricity mix calculation

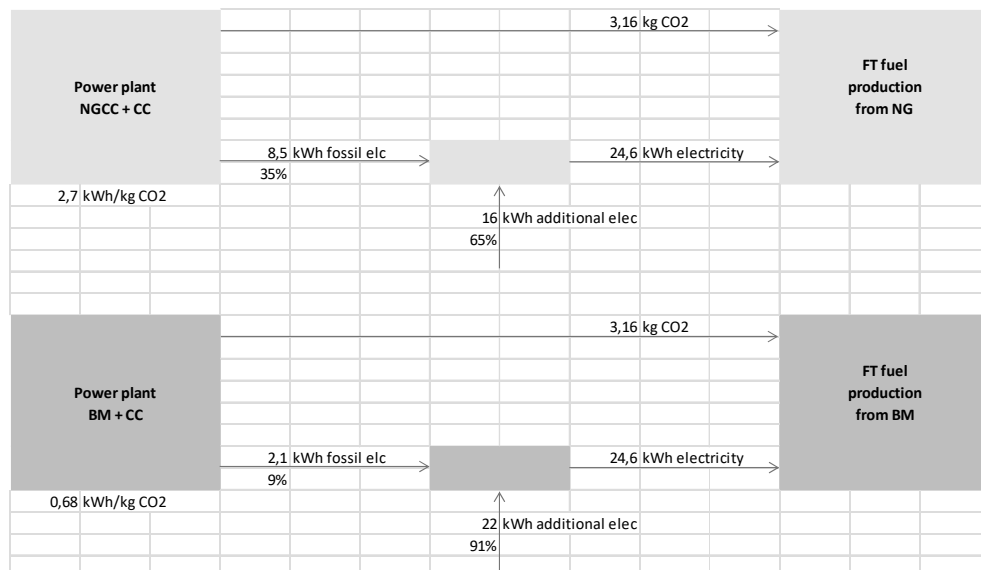


Figure 3.21: Electricity mix calculations (CO₂ demand is leading).

Syngas property calculations

Table 3.9: Blending H₂ and CO to syngas.

		M	mass	
Unit	mol	g/mol	g	%
H ₂	2	2	4	12,5%
CO	1	28	28	87,5%
Syngas	3	10,7	32	100,0%

Table 3.10: Syngas density calculation.

	0°C/1bar	230°C/25bar
M [kg/mol]	0,0107	0,0107
p [N/m ²]	100000	2500000
Z	1	1
R [Nm / (mol K)]	8,314	8,314
T [K]	273	503
density = (M x p) / (Z x R x T)	0,470	6,377

Table 3.11: Syngas LHV calculation.

	mass	LHV
	kg	MJ/kg
H ₂	0,004	120,1
CO	0,028	10,2
Syngas	0,032	23,9

Additional interpretation of LCA outcomes

Contribution of different greenhouse gases to total GHG emissions

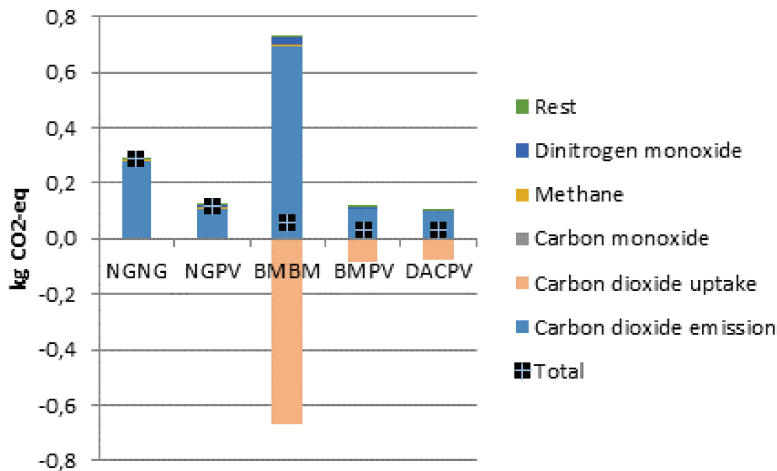


Figure 3.22: Contribution of different greenhouse gasses to net GHG emissions in kg CO₂-eq.

From Figure 3.22 it can be seen that the net GHG emissions mainly exist of carbon dioxide emissions. The uptake of carbon dioxide in the biomass alternative is higher than the uptake from the atmosphere because not all carbon dioxide that is taken up by the biomass is captured and converted into fuel again. Even the best route to produce fuels from carbon dioxide (DACPV) cannot be considered as carbon neutral, because of the emission connected to background processes.

Sensitivity analysis

Because the energy used for capturing carbon dioxide and water electrolysis is the highest contributor to the impacts a sensitivity analysis is performed to see how much a different amount of energy required for these two processes influences the end results. When the electricity demand of the electrolysis process is decreased with 10% from 56.7 kWh / kg to 51kWh / kg the impacts also decrease with 10%, making the energy demand of electrolysis an important flow (Table 3.12).

Table 3.12: Change in GWP and CED resulting from a 10% decrease in electrolysis electricity demand.

	NGNG		NGPV		BMBM		BMPV		DACPV	
	GWP	CED	GWP	CED	GWP	CED	GWP	CED	GWP	CED
Original	0,288	4,98	0,117	3,52	0,0567	7,72	0,0328	3,44	0,0296	2,85
Adjusted	0,26	4,49	0,114	3,25	0,0515	6,98	0,0302	3,16	0,0267	2,58
Change	-11%	-11%	-3%	-8%	-10%	-11%	-9%	-9%	-11%	-10%

Decreasing the CO₂ capture energy demand with 10% results in a change in electricity mix for the combustion alternatives, since more electricity per amount of carbon dioxide becomes available. Table 3.13 shows that the outcomes are hardly influenced, meaning that the energy demand for carbon dioxide capture is not the most important parameter.

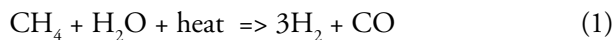
Table 3.13: Change in GWP and CED resulting from a 10% decrease in carbon capture electricity demand.

	NGNG		NGPV		BMBM		BMPV		DACPV	
	GWP	CED	GWP	CED	GWP	CED	GWP	CED	GWP	CED
Original	0,288	4,98	0,117	3,52	0,0567	7,72	0,0328	3,44	0,0296	2,85
Adjusted	0,287	4,97	0,117	3,52	0,0552	7,71	0,0314	3,44	0,0294	2,84
Change	0%	0%	0%	0%	-3%	0%	-4%	0%	-1%	0%

Producing liquid fuels from H₂ and CO₂ from SMR

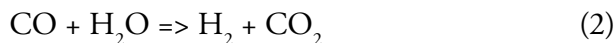
Although not starting directly from using (waste) CO₂ as a feedstock, an additional alternative to the fuel production routes in the main article might be to use hydrogen produced by steam methane reforming (SMR). The SMR process is far more efficient than using water electrolysis with renewable electricity but it emits CO₂. It is possible to capture the CO₂ emissions from SMR by using MEA based carbon scrubbing.

SMR takes place in two steps (Sumner 2006). First natural gas (methane, CH₄) and steam (water and heat) are fed to a reformer where syngas is formed (1).



It is possible to process this syngas to a Fischer-Tropsch reactor to produce liquid fuels. However gasification of natural gas gives a more beneficial H₂ : CO ratio in the syngas to be fed to the FT reactor. This is done in gas-to-liquids (GTL) being more efficient than making syngas through reforming and therefore the latter is not considered here.

The second step in SMR, is passes the resulting stream from the first reaction through a shift reaction where more steam is added and the CO and H₂O react to form more H₂ and CO₂ (2).



This CO₂ can be captured by flue gas scrubbing using MEA.

Sumner (2006) executed an LCA study on hydrogen production via steam methane reforming (SMR) with carbon capture using MEA. His system comprised of SMR unit that produces hydrogen and electricity from NG by methane reforming (see Figure 3.23).

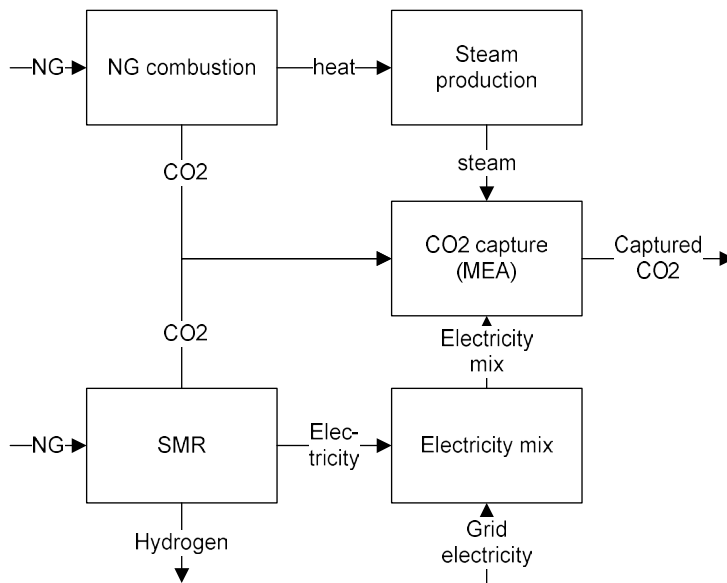


Figure 3.23: System for CO₂ and H₂ from SMR (Sumner, 2006).

Using the hydrogen and CO₂ from SMR to produce liquid fuels in the proposed route using RWGS result in 0,14 kg CO₂-eq/ MJ and 3,28 MJ / MJ. Being in the range of all other natural gas based routes presented in the main article.

For detailed LCI information we point to Sumner (2006) and the appendix of this SI (Table 3.36 - Table 3.43).

3.5.3. Life cycle inventory data of processes

Table 3.14: Electrolyser construction.

Economic inflows	Value	Unit
reinforcing steel, at plant[RER]	4,00E+03	kg
disposal, building, fibre board, to final disposal[CH]	51	kg
disposal, building, bulk iron (excluding reinforcement), to sorting plant[CH]	8,00E+03	kg
chromium steel 18/8, at plant[RER]	8,00E+03	kg
transport, freight, rail[RER]	2,55E+03	tkm
nitrogen, liquid, at plant[RER]	85	kg
potassium hydroxide, at regional storage[RER]	30	kg
sodium silicate, spray powder 80%, at plant[RER]	200	kg
corrugated board, recycling fibre, double wall, at plant[RER]	51	kg
disposal, building, reinforcement steel, to sorting plant[CH]	4,00E+03	kg
transport, lorry 16-32t, EURO3[RER]	1,23E+03	tkm
Economic outflows		
Electrolyser for hydrogen production	1	unit
Environmental resources		
Occupation, industrial area, built up[resource_land]	29,8	m2a
Environmental emissions		
Hydrogen[air_unspecified]	5,36	kg

Table 3.15: Hydrogen production, electrolysis.

Economic inflows	Value	Unit
tap water, at user[RER]	11,1	kg
Electrolyser for hydrogen production	2,31E-06	unit
Electricity mix	56,7	kWh
Economic outflows		
Hydrogen gas from electrolysis (NG NG)	1	kg
Environmental resources		
-		
Environmental emissions		
-		

Table 3.16: Hydrogen compressor construction.

Economic inflows	Value	Unit
steel, low-alloyed, at plant[RER]	3,00E+03	kg
disposal, building, concrete, not reinforced, to sorting plant[CH]	2,60E+04	kg
aluminium, production mix, at plant[RER]	500	kg
concrete, normal, at plant[CH]	12	m3
disposal, building, bulk iron (excluding reinforcement), to sorting plant[CH]	8,00E+03	kg
chromium steel 18/8, at plant[RER]	5,00E+03	kg
lubricating oil, at plant[RER]	150	kg
transport, freight, rail[RER]	1,79E+03	tkm
disposal, aluminium, 0% water, to municipal incineration[CH]	500	kg
transport, lorry 16-32t, EURO3[RER]	2,16E+03	tkm
Economic outflows		
Hydrogen compressor	1	unit
Environmental resources		
Occupation, industrial area, built up[resource_land]	16,2	m2a
Environmental emissions		
-		

Table 3.17: Hydrogen compression to 25 bar.

Economic inflows	Value	Unit
Hydrogen compressor	3,42E-08	unit
NGNG based electricity mix	0,66	kWh
Hydrogen gas from electrolysis	1	kg
Economic outflows		
Hydrogen gas @ 25 bar	1	kg
Environmental resources		
-		
Environmental emissions		
-		

Table 3.18: RWGS catalyst production.

Economic inflows	Value	Unit
copper oxide, at plant[RER]	0,57	kg
aluminium oxide, at plant[RER]	0,11	kg
zinc oxide, at plant[RER]	0,31	kg
Economic outflows		
RWGS catalyst	1	kg
Environmental resources		
-		
Environmental emissions		
-		

Table 3.19: Fixed bed reactor construction.

Economic inflows	Value	Unit
steel, low-alloyed, at plant[RER]	4,76E+03	kg
disposal, building, bulk iron (excluding reinforcement), to sorting plant[CH]	9,52E+03	kg
chromium steel 18/8, at plant[RER]	4,76E+03	kg
zeolite, powder, at plant[RER]	2,67E+04	kg
RWGS catalyst	6,60E+03	kg
Economic outflows		
Fixed bed reactor for RWGS	1	unit
Environmental resources		
Occupation, industrial area[resource_land]	3,14	m2a
Environmental emissions		
-		

Table 3.20: CO production via RWGS.

Economic inflows	Value	Unit
Fixed bed reactor for RWGS	1,93E-09	unit
CO2 from NGCC @25 bar	1,57	kg
Hydrogen gas @ 25 bar	0,07	kg
Economic outflows		
Carbon Monoxide from RWGS	1	kg
Environmental resources		
-		
Environmental emissions		
-		

Table 3.21: Syngas production.

Economic inflows	Value	Unit
Hydrogen gas @ 25 bar	0,125	kg
Carbon Monoxide from RWGS	0,875	kg
Economic outflows		
Syngas	1	kg
Environmental resources		
-		
Environmental emissions		
-		

Table 3.22: GTL plant construction.

Economic inflows	Value	Unit
concrete, sole plate and foundation, at plant[CH]	3,45E+05	m3
steel, low-alloyed, at plant[RER]	7,20E+06	kg
reinforcing steel, at plant[RER]	7,20E+06	kg
disposal, building, reinforced concrete, to final disposal[CH]	8,28E+08	kg
disposal, building, bulk iron (excluding reinforcement), to sorting plant[CH]	1,44E+07	kg
Economic outflows		
GTL plant	1	unit
Environmental resources		
Occupation, industrial area[resource_land]	1,12E+06	m2a
Environmental emissions		
x	x	x

Table 3.23: Syngas production.

Economic inflows	Value	Unit
Syngas	2,3	kg
GTL plant	6,70E-12	unit
Economic outflows		
GTL product	1	kg
Environmental resources		
-		
Environmental emissions		
-		

Table 3.24: natural gas, burned in combined cycle plant, best technology, with carbon capture + compression.

Economic inflows	Value	Unit
water, decarbonised, at plant[RER]	0,5	kg
hydrochloric acid, 30% in H ₂ O, at plant[RER]	2,50E-06	kg
sodium hydroxide, 50% in H ₂ O, production mix, at plant[RER]	2,00E-06	kg
natural gas, high pressure, at consumer[RER]	1	MJ
disposal, residue from cooling tower, 30% water, to sanitary landfill[CH]	1,00E-06	kg
gas combined cycle power plant, 400MWe[RER]	2,20E-12	unit
Economic outflows		
natural gas, burned in combined cycle plant, with carbon capture[RER]	1	MJ
Carbon dioxide from NGCC before capture	0,056	kg
Environmental resources		
Heat, waste[air_high population density]	0,525	MJ
Nitrogen oxides[air_high population density]	2,55E-05	kg
Particulates, < 2.5 um[air_high population density]	5,00E-07	kg
Carbon monoxide, fossil[air_high population density]	2,20E-06	kg
Dinitrogen monoxide[air_high population density]	1,00E-06	kg
Acetic acid[air_high population density]	1,21E-07	kg
Methane, fossil[air_high population density]	1,00E-06	kg
Sulfur dioxide[air_high population density]	5,00E-07	kg
Toluene[air_high population density]	1,50E-09	kg
Acetaldehyde[air_high population density]	8,00E-10	kg
Propane[air_high population density]	7,05E-07	kg
Propionic acid[air_high population density]	1,60E-08	kg
Formaldehyde[air_high population density]	3,31E-08	kg
Benzene[air_high population density]	9,26E-10	kg
Benzo(a)pyrene[air_high population density]	5,29E-13	kg
Dioxins, measured as 2,3,7,8-tetrachlorodibenzo-p-dioxin [air_high population density]	2,90E-17	kg
Mercury[air_high population density]	3,00E-11	kg
PAH, polycyclic aromatic hydrocarbons[air_high population density]	8,00E-09	kg
Butane[air_high population density]	9,26E-07	kg
Pentane[air_high population density]	1,15E-06	kg
Ethane[air_high population density]	1,37E-06	kg
Hexane[air_high population density]	7,93E-07	kg
Acenaphthene[air_high population density]	7,93E-13	kg

Table 3.25: electricity, natural gas, at combined cycle plant, best technology, with carbon capture and compression.

Economic inflows	Value	Unit
natural gas, burned in combined cycle plant, with carbon capture	7,36	MJ
Economic outflows		
electricity, natural gas, at combined cycle plant, with carbon capture	1	kWh
Environmental resources		
-		
Environmental emissions		
-		

Table 3.26: Carbon capture + compression to 25 bar.

Economic inflows	Value	Unit
tap water, at user[RER]	216	kg
monoethanolamine, at plant[RER]	1,6	kg
Carbon dioxide from NGCC before capture	1,11E+03	kg
CO ₂ capture + compression plant for NGCC power plant	3,30E-08	unit
Economic outflows		
CO ₂ from NGCC @25 bar	1,00E+03	kg
Environmental resources		
-		
Environmental emissions		
Heat, waste[air_low population density]	855	MJ
Carbon dioxide, fossil[air_high population density]	111	kg
Heat, waste[water_unspecified]	3,41E+03	MJ

Table 3.27: CO₂ capture plant + compressor construction.

Economic inflows	Value	Unit
steel, low-alloyed, at plant[RER]	3,91E+06	kg
disposal, building, bulk iron (excluding reinforcement), to sorting plant[CH]	4,86E+06	kg
chromium steel 18/8, at plant[RER]	9,48E+05	kg
Economic outflows		
CO ₂ capture + compression plant for NGCC power plant	1	unit
Environmental resources		
Transformation, from unknown[resource_land]	4,00E+04	m2
Occupation, industrial area[resource_land]	1,44E+06	m2a
Transformation, to industrial area[resource_land]	4,00E+04	m2
Environmental emissions		
-		

Table 3.28: wood chips, burned in power plant with carbon capture.

Economic inflows	Value	Unit
transport, lorry >16t, fleet average[RER]	0,00013	tkm
transport, freight, rail[RER]	0,000351	tkm
water, decarbonised, at plant[RER]	0,15	kg
chlorine, liquid, production mix, at plant[RER]	1,00E-05	kg
disposal, residue from cooling tower, 30% water, to sanitary landfill[CH]	5,00E-06	kg
light fuel oil, at regional storage[RER]	1,70E-05	kg
water, completely softened, at plant[RER]	0,006	kg
hard coal power plant[RER]	1,30E-12	unit
SOx retained, in hard coal flue gas desulphurisation[RER]	0,000118	kg
NOx retained, in SCR[GLO]	3,09E-05	kg
disposal, hard coal ash, 0% water, to residual material landfill[ES]	0,00651	kg
Wood chips from short-rotation wood	0,068	kg
Economic outflows		
wood chips, burned in power plant with carbon capture[ES]	1	MJ
Carbon dioxide from biomass combustion before capture	0,121	kg
Environmental resources		
Water, cooling, unspecified natural origin[resource_in water]	0,0035	m3
Environmental emissions		
Heat, waste[air_low population density]	0,548	MJ
Dinitrogen monoxide[air_low population density]	8,90E-07	kg
Nitrogen oxides[air_low population density]	0,000362	kg
Carbon monoxide, fossil[air_low population density]	8,00E-06	kg
Sulfur dioxide[air_low population density]	0,000731	kg
Methane, fossil[air_low population density]	1,00E-06	kg
Benzene[air_low population density]	2,17E-07	kg
Particulates, < 2.5 um[air_low population density]	4,85E-05	kg
Cadmium[air_low population density]	4,47E-10	kg
Chromium[air_low population density]	4,23E-09	kg
Copper[air_low population density]	6,07E-09	kg
Nickel[air_low population density]	1,19E-08	kg
Zinc[air_low population density]	4,13E-08	kg
Benzo(a)pyrene[air_low population density]	2,00E-13	kg
PAH, polycyclic aromatic hydrocarbons[air_low population density]	1,00E-09	kg
Selenium[air_low population density]	7,95E-09	kg
Lead[air_low population density]	2,64E-08	kg
Particulates, > 10 um[air_low population density]	7,85E-06	kg

Hydrogen fluoride[air_low population density]	4,23E-06	kg
Particulates, > 2.5 um, and < 10um[air_low population density]	5,70E-06	kg
Uranium-238[air_low population density]	1,57E-05	kBq
Thorium-228[air_low population density]	3,10E-06	kBq
Radium-226[air_low population density]	1,88E-05	kBq
Radon-222[air_low population density]	0,000582	kBq
Lead-210[air_low population density]	7,29E-05	kBq
Polonium-210[air_low population density]	0,000133	kBq
Potassium-40[air_low population density]	1,43E-05	kBq
Thorium-232[air_low population density]	4,87E-06	kBq
Heat, waste[water_river]	0,144	MJ
Antimony[air_low population density]	5,36E-10	kg
Arsenic[air_low population density]	7,63E-09	kg
Barium[air_low population density]	5,10E-08	kg
Boron[air_low population density]	6,51E-07	kg
Bromine[air_low population density]	2,94E-07	kg
Butane[air_low population density]	1,90E-08	kg
Chromium VI[air_low population density]	5,23E-10	kg
Cobalt[air_low population density]	2,18E-09	kg
Dioxins, measured as 2,3,7,8-tetrachlorodibenzo-p-dioxin[air_low population density]	7,00E-15	kg
Ethane[air_low population density]	4,10E-08	kg
Formaldehyde[air_low population density]	5,80E-08	kg
Hydrocarbons, aliphatic, alkanes, unspecified[air_low population density]	2,19E-07	kg
Hydrocarbons, aliphatic, unsaturated[air_low population density]	2,16E-07	kg
Hydrogen chloride[air_low population density]	1,31E-05	kg
Iodine[air_low population density]	1,35E-07	kg
Manganese[air_low population density]	1,33E-08	kg
Mercury[air_low population density]	5,16E-09	kg
Molybdenum[air_low population density]	8,72E-10	kg
Pentane[air_low population density]	1,47E-07	kg
Propane[air_low population density]	3,50E-08	kg
Propene[air_low population density]	1,60E-08	kg
Radium-228[air_low population density]	5,76E-06	kBq
Radon-220[air_low population density]	0,000327	kBq
Strontium[air_low population density]	7,04E-08	kg
Toluene[air_low population density]	1,09E-07	kg
Vanadium[air_low population density]	1,24E-08	kg
Xylene[air_low population density]	9,22E-07	kg

Table 3.29: electricity, wood pellets, power plant with carbon capture.

Economic inflows	Value	Unit
wood chips, burned in power plant with carbon capture[ES]	13,5	MJ
Economic outflows		
electricity, wood chips at power plant with carbon capture	1	kWh
Environmental resources		
-		
Environmental emissions		
-		

Table 3.30: CO₂ capture plant for biomass power plant.

Economic inflows	Value	Unit
steel, low-alloyed, at plant[RER]	6,11E+06	kg
disposal, building, bulk iron (excluding reinforcement), to sorting plant[CH]	7,58E+06	kg
chromium steel 18/8, at plant[RER]	1,47E+06	kg
Economic outflows		
CO ₂ capture plant for Biomass power plant	1	unit
Environmental resources		
Transformation, from unknown[resource_land]	4,20E+04	m2
Occupation, industrial area[resource_land]	1,44E+06	m2a
Transformation, to industrial area[resource_land]	4,20E+04	m2
Environmental emissions		
-		

Table 3.31: Carbon capture + compression from biomass power plant.

Economic inflows	Value	Unit
tap water, at user[RER]	262	kg
monoethanolamine, at plant[RER]	1,6	kg
Carbon dioxide from biomass combustion before capture	1,11E+03	kg
CO ₂ capture plant for Biomass power plant	1,24E-08	unit
Economic outflows		
CO ₂ from BM @25 bar	1,00E+03	kg
Environmental resources		
-		
Environmental emissions		
Heat, waste[air_low population density]	744	MJ
Carbon dioxide, fossil[air_high population density]	111	kg
Heat, waste[water_unspecified]	4,25E+03	MJ

Table 3.32: Direct air capture (DAC) equipment.

Economic inflows	Value	Unit
steel, low-alloyed, at plant[RER]	3,80E+03	kg
disposal, building, bulk iron (excluding reinforcement), to sorting plant[CH]	3,80E+03	kg
Economic outflows		
DAC equipment (absorber)	1	unit
Environmental resources		
Occupation, industrial area[resource_land]	36	m2a
Environmental emissions		
-		

Table 3.33: Direct air capture.

Economic inflows	Value	Unit
electricity, production mix photovoltaic, at plant[ES]	0,31	kWh
DAC equipment (absorber)	9,13E-08	unit
Economic outflows		
CO ₂ from direct air capture @25 bar	1	kg
Environmental resources		
Carbon dioxide, in air[resource_in air]	1	kg
Environmental emissions		
-		

Table 3.34: Electricity mix.

Economic inflows	Value	Unit
electricity, source A	0,65	kWh
electricity, source B	0,35	kWh
Economic outflows		
electricity mix	1	kWh
Environmental resources		
-		
Environmental emissions		
-		

Table 3.35: SMR construction.

Economic inflows	Value	Unit
steel, low-alloyed, at plant[RER]	3.01E6	kg
disposal, building, concrete, not reinforced, to sorting plant[CH]	9.42E6	kg
concrete, normal, at plant[CH]	4.28E3	m3
disposal, building, bulk iron (excluding reinforcement), to sorting plant[CH]	3.05E6	kg
transport, freight, rail[RER]	6.15E5	tkm
aluminium, primary, at plant[RER]	2.48E4	kg
pig iron, at plant[GLO]	3.68E4	kg
disposal, aluminium, 0% water, to municipal incineration[CH]	2.48E4	kg
transport, lorry >32t, EURO4[RER]	7.79E5	tkm
Economic outflows		
Steam methane reformer	1	unit
Environmental resources		
Occupation, industrial area[resource_land]	2.25E4	m2a
Environmental emissions		
-		

Table 3.36: Steam methane Reforming.

Economic inflows	Value	Unit
tap water, at user[RER]	10.9	kg
natural gas, high pressure, at consumer[RER]	183	MJ
Steam methane reformer	9.21E-10	unit
Economic outflows		
CO ₂ to amine fluegas scrubbing	9.23	kg
Hydrogen gas from SMR + CC	1	kg
Electricity, med V, from SMR + CC	2.98	kWh
Environmental resources		
Water, cooling, unspecified natural origin[resource_in water]	0.0286	m3
Environmental emissions		
Carbon dioxide, fossil[air_low population density]	1.02	kg
Nitrogen oxides[air_low population density]	0.00475	kg
Particulates, < 2.5 um[air_unspecified]	2.2E-5	kg
Carbon monoxide, biogenic[air_low population density]	7.98E-5	kg

Table 3.37: Natural gas, burned in industrial furnace >100kW, with carbon capture.

Economic inflows	Value	Unit
electricity, low voltage, production UCTE, at grid[UCTE]	0.00111	kWh
natural gas, high pressure, at consumer[RER]	1	MJ
industrial furnace, natural gas[RER]	2.8E-9	unit
Economic outflows		
CO ₂ to amine fluegas scrubbing	0.0504	kg
Natural gas, burned in industrial furnace >100kW, with carbon capture[RER]	1	MJ
Environmental resources		
-		
Environmental emissions		
Carbon dioxide, fossil[air_low population density]	1.02	kg
Nitrogen oxides[air_low population density]	0.00475	kg
Heat, waste[air_high population density]	1.1	MJ
Nitrogen oxides[air_high population density]	1.79E-5	kg
Particulates, < 2.5 um[air_high population density]	2,00E-07	kg
Carbon monoxide, fossil[air_high population density]	2.1E-6	kg
Carbon dioxide, fossil[air_high population density]	0.0056	kg
Dinitrogen monoxide[air_high population density]	1,00E-07	kg
Acetic acid[air_high population density]	1.5E-7	kg
Methane, fossil[air_high population density]	2,00E-06	kg
Sulfur dioxide[air_high population density]	5.5E-7	kg
Toluene[air_high population density]	2,00E-07	kg
Acetaldehyde[air_high population density]	1,00E-09	kg
Propane[air_high population density]	2,00E-07	kg
Propionic acid[air_high population density]	2,00E-08	kg
Formaldehyde[air_high population density]	1,00E-07	kg
Benzene[air_high population density]	4,00E-07	kg
Benzo(a)pyrene[air_high population density]	1,00E-11	kg
Dioxins, measured as 2,3,7,8-tetrachlorodibenzo-p-dioxin[air_high population density]	3,00E-17	kg
Mercury[air_high population density]	3,00E-11	kg
PAH, polycyclic aromatic hydrocarbons[air_high population density]	1,00E-08	kg
Butane[air_high population density]	7,00E-07	kg
Pentane[air_high population density]	1.2E-6	kg

Table 3.38: Steam production from NG for carbon capture.

Economic inflows	Value	Unit
tap water, at user[RER]	1.17	kg
Natural gas, burned in industrial furnace >100kW, with carbon capture[RER]	3.23	MJ
Economic outflows		
Steam for carbon capture	1	kg
Environmental resources		
-		
Environmental emissions		
-		

Table 3.39: Steam production from NG for carbon capture.

Economic inflows	Value	Unit
steel, low-alloyed, at plant[RER]	9.02E8	kg
bitumen, at refinery[CH]	1.1E6	kg
disposal, building, concrete, not reinforced, to sorting plant[CH]	5.96E6	kg
concrete, normal, at plant[CH]	2.71E3	m3
disposal, building, bulk iron (excluding reinforcement), to sorting plant[CH]	9.18E5	kg
disposal, bitumen, 1.4% water, to sanitary landfill[CH]	1.1E6	kg
transport, freight, rail[RER]	8.44E5	tkm
transport, lorry >32t, EURO4[RER]	5,00E+05	tkm
Economic outflows		
Carbon scrubber	1	unit
Environmental resources		
-		
Environmental emissions		
-		

Table 3.40: Carbon scrubbing from SMR and steam generation.

Economic inflows	Value	Unit
tap water, at user[RER]	2.49	kg
monoethanolamine, at plant[RER]	0.002	kg
CO2 to amine fluegas scrubbing	1	kg
Steam for carbon capture	1.39	kg
Hydrogen compressor (James)	4.23E-7	unit
Carbon scrubber	1.16E-10	unit
mixed electricity at SMR plant	0.132	kWh
Economic outflows		
CO2 from SMR and Steam gen	1	kg
Environmental resources		
-		
Environmental emissions		
Monoethanolamine[air_high population density]	0.001	kg

Table 3.41: Electricity mixing for Carbon scrubbing (SMR).

Economic inflows	Value	Unit
electricity, medium voltage, production UCTE, at grid[UCTE]	0.525	kWh
Electricity, med V, from SMR + CC	0.475	kWh
Economic outflows		
mixed electricity at SMR plant	1	kWh
Environmental resources		
-		
Environmental emissions		
-		

Table 3.42: Hydrogen (SMR +CC) compression.

Economic inflows	Value	Unit
Hydrogen gas from SMR + CC	1	kg
Hydrogen compressor (James)	4.23E-7	unit
mixed electricity at SMR plant	0.223	kWh
Economic outflows		
Hydrogen (SMR+CC) @ 25 bar	1	kg
Environmental resources		
-		
Environmental emissions		
-		

