

BeKind

Circularity and climate benefit of a <u>b</u>io- and <u>e</u>lectro-based <u>c</u>hemical <u>ind</u>ustry - effects of transitions in petrochemical value chains

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Rapportnummer C 722 ISBN 978-91-7883-451-8 Upplaga Finns endast som PDF-fil för egen utskrift

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Preface

This document reports the finding from the project BeKind: Circularity and climate benefit of a Bio- and Electro-based Chemical Industry - effects of transitions in petrochemical value chains. The aim of the BeKind-project has been to identify challenges for transition to a circular and climate-neutral petrochemical industry, to develop proposals for remedial activities for these obstacles and challenges, and to quantify the benefits such a transition can have for circularity, climate and social sustainability. The focus of the project has been on industrial production of liquid fuels and plastics.

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Sammanfattning

Syftet med BeKind-projektet är att identifiera hinder och utmaningar för omställning till en cirkulär och klimatneutral petrokemisk industri, ta fram förslag på avhjälpande aktiviteter för dessa hinder och utmaningar, samt att kvantifiera de nyttor en sådan omställning kan få för cirkularitet, klimat och social hållbarhet. Fokus för projektet ligger på industriell produktion av flytande bränslen och plaster.

När omställningen av den petrokemiska industrisektorn genomförs kommer nya värdekedjor etableras som gör att sektorer och industriaktörer som inte tidigare samarbetat börjar interagera. Studien bygger på ett scenario där delar av industrin elektrifieras men där den primära kolkällan är förnybara oljor, i form av bio-, retur-, och elektrosyntesoljor (bio-crude, retur-crude, resp. elektro-crude). Det vill säga icke-raffinerade primärprodukter från en pyrolys- respektive elektrosyntes-process samt resultatet av återvunna fraktioner från kemiskt återvunnen plast. Projektet genomförs i en konstellation med forskare och industriaktörer som i huvudsak representerar värdekedjan bio/retur/elektro-olja \rightarrow raffinaderi \rightarrow kemiindustri.

Denna studie har fyra huvudsakliga mål:

- 1. Kartlägga hinder och utmaningar för de industrisektorer som ingår i de värdekedjor som ingår i studien.
- 2. Beskriva förslag på avhjälpande aktiviteter för att överbrygga hinder och utmaningar i samråd med berörda industrisektorer.
- 3. Beräkna mass- och energibalanser för de inkluderade värdekedjorna.
- 4. Kvantifiera cirkularitets- och klimatnyttan och genomföra social hållbarhetsbedömning för de nya värdekedjorna jämfört med befintliga, fossila dito.

Övergången till en cirkulär och klimatneutral petrokemisk industri innebär utmaningar på flera plan eftersom företag från olika branscher som inte har samarbetat tidigare kommer att behöva samarbeta. I denna rapport ligger fokus på samverkan och samordning, ekonomiska och organisatoriska utmaningar. Det visar sig att ett stort arbete måste utföras när det gäller att bilda partnerskap och plattformar där utmaningarna kan hanteras. Aktörerna måste hantera och nå överenskommelser kring praktiska frågor som kvalitetsspecifikation, logistik och kontraktslängder En gemensam grundförståelse för hållbarhet måste hittas. För att kunna dela riskerna kopplade till de investeringar som krävs och garantera en långsiktig utveckling behöver mer formaliserade former av partnerskap och joint ventures grundas. Lagstiftning och regelverk behöver även finnas på plats och ha en tydlighet för de berörda aktörerna.

De mass- och energibalanser som presenteras här är baserade på en litteraturgenomgång som inkluderade både vetenskapliga artiklar och relevanta rapporter. Dessa mass- och energi-balanser innefattar de processer som ingår i omvandlingar och vidareförädling från råvara till slutprodukt, dvs. metanol, FT-crude och pyrolysolja. Den mängd råvara och det totala energibehovet normaliserades per kg slutprodukt. Analysen visar att, med utgångspunkt från CO₂ och H₂ som råmaterial, så är metanol mindre materialintensiv än produktion av FT-crude. Det betyder att med samma mängd råmaterial, så producerar man mer metanol än FT-crude. I de fall där skogsavfall används som råmaterial var FT-crude något mindre materialintensivt. Energibalanserna i alla värdekedjor inkluderade någon form av energiintegration med en annan industri (industriell symbios) eller hade en värmeåtervinningsångcykel, vilket minskade energibehovet avsevärt. De

mest energikrävande processerna var produktionen av väte genom elektrolys och den omvända vattengasskifte-reaktionen.

Bedömningen av cirkularitetsnyttan av olika värdekedjor gjordes genom att använda en metod som utvecklas i ett tidigare IVLs projekt, "Security of supply and circularity of transport biofuels -Method development." (Lönnqvist, et al., 2022). Bedömningsmetoden är baserad på andelen förnybart-och återvunnet material som används som material-och energiinsatst i respektive värdekedja. Att förnybart ursprung och andel återvunnet material används speglar det "cirkulära" ursprunget av insatsvarorna till en produkt snarare än hur många gånger produkten kan cirkulera i systemet. Detta innebär således att den vanliga tolkningen av cirkularitet dvs. förlustminimering och slutna system inte appliceras i metoden. Istället undersöker detta projekt en annan betydelse av cirkularitet genom att titta på hur material med lågt värde tas tillvara och uppgraderas till ett annat material med högre kvalitet och värde.

Analysen visar att FT-crude och metanol från skogsrester är 79% respektive 89% cirkulärt vilket är högre än värdekedjorna av elektrobränsle. De värdekedjor som är baserade på elektrobränslen, FTcrude och metanol från CO₂ och H₂, har 78% cirkularitet. Pyrolysolja från plastavfall har lägst cirkularitetsindex på 51% Trots att plastavfall hade 100% andel återvunnet material. Detta är eftersom plastavfallet innehåller endast 1-2% förnybart material vilket leder till att cirkularitetsindexen sänktes avsevärt. Cirkularitetsindex för metanol från skogsrester var 83% vilket innebär att cirkularitetsnyttan av den värdekedjan är högst då siffran på cirkularitetsindex tyder på att råmaterial som har låg kvalitet kan effektivt uppgraderas till en produkt med högre kvalitet.

Resultatet från klimatpåverkansbedömningen visar på en potentiell klimatnytta genom nyttjandet av förnybara råvaror i kemiindustrin (såsom skogsrester och infångad koldioxid från förnybara råvaror) i förhållande till fossila råmaterial (såsom råolja och naturgas). Detta gäller för både metanol och FT crude som tillverkas från förnybara råvaror. Det gick inte att utläsa någon potentiell klimatnytta från produktion och användning av pyrolysolja från plastavfall i denna studie eftersom det fossila råmaterialet ger upphov till koldioxidutsläpp både från spill vid återvinningen och vid end-of-life. Energiintegration eller industriell symbios för produktionsprocesser för förnybara råmaterial sänker ytterligare deras klimatpåverkan genom att det externa energibehovet minskar.

I resultatet från den sociala hållbarhetsbedömningen kan man utläsa att införandet av nya råmaterial till kemiindustrin kan utgöra nya och okända risker inom arbetsmiljön, speciellt då råmaterialen som används idag främst är i flytande eller gasform snarare än fasta såsom skogsrester. Angående jobbtillfällen kan man dra slutsatsen att nya jobbtillfällen kan uppstå som processoperatörer, underhållsoperatörer och lastbilschaufförer vid införandet av nya råmaterial till kemiindustrin. Den sociala hållbarhetsbedömningen genomfördes under en workshop tillsammans med projektpartners.

Summary

The aim of the BeKind-project is to identify obstacles and challenges for transition to a circular and climate-neutral petrochemical industry, to develop proposals for remedial activities for these obstacles and challenges, and to quantify the benefits such a transition can have for circularity, climate and social sustainability. The focus of the project is on industrial production of liquid fuels and plastics.

When the restructuring of the petrochemical industrial sector is carried out, new value chains will be established, which will mean that sectors and industrial actors that have not previously collaborated will begin to interact. The study is based on a scenario where parts of the industry are electrified but where the primary source of coal is renewable oils, in the form of bio-, recycled and electro-synthesized oils (bio-crude, recycled-crude, or electro-crude), i.e., unrefined primary products from a pyrolysis or electrosynthesis process and the result of chemically recycled plastics. The project is carried out in a constellation with researchers and industrial actors who, for the most part, represent the value chain bio / recycled / electro-oil \rightarrow refinery \rightarrow chemical industry.

This study has four main objectives:

- 1. Identify obstacles and challenges for the industrial sectors involved in or affected by the new value chains in focus of the study.
- 2. Describe proposals for remedial activities to overcome obstacles and challenges in consultation with relevant industrial sectors.
- 3. Calculate mass and energy balances for the included value chains.
- 4. Quantify the degree of circularity and climate benefits and carry out social sustainability assessment for the new value chains compared to existing fossil fuel based processes and value chains.

In this report the focus is on collaboration and coordination, financial and organizational challenges. It is found that a great amount of work needs to be performed in terms of forming partnership and platforms where the challenges can be handled. Practical issues such as quality specification, logistics and lengths of contracts need to be agreed upon. A common ground for sustainability needs to be found. To collectively share risks of investments and to guarantee a long-term development new forms of partnerships and joint ventures need to be formed. Laws and regulations also needs to be put in place and and formulated in a way that creates clarity for the stakeholders that are affected by them.

Mass and energy balances were collected through a literature review including scientific papers and relevant reports. The mass and energy balances include all processes from feedstock supply to final product in the form of methanol, FT-crude and pyrolysis oil. The amount of feedstock and the overall energy demand were normalized per kg of final product. The assessment shows that, starting from CO₂ and H₂ as feedstock, methanol is less material intensive than FT-crude production. This means that starting from the same amount of raw materials, methanol will be produced in larger quantity than FT-crude. When starting from forest residues, FT-crude was slightly less material intensive. The energy balances of all value chains included some kind of energy integration with another industry (industrial symbiosis) or had a heat recovery steam cycle, which considerably reduced the energy demands. The most energy demanding processes were the production of hydrogen via electrolysis and the reverse water gas shift reaction. C

The evaluation of the circularity benefits of different value chains was carried out by adopting a method which was developed in aprevious project at IVL called "*Security of supply and circularity of transport biofuels – Method development*" (Lönnqvist, et al., 2022). The circularity evaluation method is based on the share of renewable material and recycled content of all material and energy inputs in the value chain. The use of renewable origin and the share of recycled material as indicators in the method reflect the share of inputs with "circular" origin in the production of a product rather than showing how many times the product can be circulated in a system. Thus, the normal perception of circular economy i.e. waste minimisation and creating a closed system is not applied in the method. Instead, the project investigates another meaning of circularity by looking at how material with low quality can be upcycled to a higher value product.

The evaluation shows that forest residue-based FT-crude and methanol have a circularity score of 79% and 83% respectively, which are higher than the value chains of electrofuels. The electrofuel i.e. the FT-crude and methanol from biogenic CO₂ and H₂ have a circularity score of about 78%. The pyrolysis oil from plastic waste shows the lowest circularity score of 51% albeit the 100% recycled fraction. This can be explained by the fact that the plastic waste available in Sweden is estimated to contain only 1-2% of renewable material, which in turn decrease the circularity score of the pyrolysis oil considerably. The highest circularity score (83%) of methanol from forest residue implies the highest circularity benefit as the score indicates that the value chain can efficiently upcycle the low-quality inputs to a higher quality output.

In the climate impact assessment, a potential climate benefit could be identified when using renewable raw materials (forest residues and captured carbon dioxide) instead of continued use offossil raw material (crude oil and natural gas). This was the case for both methanol and FT crude. It was not possible to identify, in this assessment, a climate benefit when using pyrolysis oil from plastic waste compared to naphtha from crude oil, since a fossil raw material such as plastic waste generates carbon dioxide emissions from production waste and at the end-of-life. Energy integration of the production processes for renewable materials further decreases the climate impact.

The results from the social sustainability assessment showed that introduction of new raw materials to the chemical industry could pose new and unknown risks in the working environment, especially since the materials used today often are liquids or gaseous rather than solid materials such as forest residues. With regards to job opportunities, it was concluded that new job opportunities could appear as process operators, maintenance operators and lorry drivers when introducing new raw materials for the chemical industry. The social sustainability assessment was performed as a workshop for project partners.

1 Introduction

The focus of the project is on the industrial production of liquid fuels and plastics. The study is based on a scenario where parts of the industry are electrified but where the primary carbon source is renewable and circular oils, in the form of bio-, recycled and electrosynthesized oils (bio-crude, recycled-crude, or electro-crude). I.e., unrefined primary products from a pyrolysis or electrosynthesis process and the result of chemically recycled plastics. The project is carried out in a constellation with researchers and industrial actors representing the value chain: bio/return/electro-oil \rightarrow refinery \rightarrow chemical industry.

This study has four main objectives:

- 1. Map obstacles and challenges for industrial sectors affected by the new value chains. When the restructuring of the petrochemical industry sector is carried out, new value chains will be established which will require sectors and industry actors that have not previously cooperated to begin to interact. What the collaborations will look like and how well they will function is uncertain at this point. Obstacles and challenges can, for example, consist of:
 - a. Organizational obstacles in new collaborations, e.g., in the form of different time perspectives on investments,
 - b. Policy, laws and regulations look different for the different sectors and can differ between countries,
 - c. Potential goal conflicts which can arise when sectors link their value chains and establish frequent exchanges, e.g., between forest and petrochemical industry.
- 2. Describe proposals for remedial activities to overcome obstacles and challenges. In consultation with the relevant industry sectors, proposals are drawn up for strategies and activities that have the potential to remedial obstacles and challenges.
- 3. Calculate mass and energy balances for the included value chains, including upstream and downstream of the refinery, as well as distribution in the refining process.
- 4. Quantify circularity and climate benefit and carry out social sustainability assessment for the new value chains relative to existing, fossil ditto.

The reference value is the existing fossil-based production system. The three different raw material streams will have different benefits in terms of climate and circularity, which is valuable knowledge for future path choices regarding carbon sources for the petrochemical industry. Furthermore, the results can be used to show what benefits a restructuring of the petrochemical industry brings to society, which in turn can be the basis for a discussion about incentives. The long-term benefit of the project is to contribute to: i) climate-neutral and circular production, ii) resource-efficient and resilient value chains, iii) a socially sustainable industry, and iv) global competitiveness. Also, the project has a high degree of industrial symbiosis through the integration of residual products in the form of forest residues, biogenic carbon dioxide and collected plastic from relevant industrial sectors in existing processes in the petrochemical industry and downstream into new high-value products. All project partners want to increase their understanding of the obstacles and challenges that can arise when industry sectors must cooperate in new ways and how they can be remedied. And all partners have contributed with their own experiences/perspectives on the transition, which are thus collected and addressed in the project.

2 Background

The Swedish petrochemical industry includes different types of companies with different product portfolios and varying production processes. The companies are in many cases relatively large and foreign-owned and mainly operate around the metropolitan regions and along the northeastern coast. The sector is highly dependent on exports (>85%) and thus competes on global markets. The export value is around SEK 160 billion (IVA, 2019), which corresponds to around 12 percent of Sweden's GDP. The sector thus creates value for the Swedish economy at the same time as it uses approximately 12 TWh of energy annually (Energy Agency, 2018), of which almost 60 percent is of fossil origin. The Swedish chemical industry and the Swedish refineries currently release 1.3 and 2.9 million tonnes of greenhouse gases respectively annually (SCB, 2018). The petrochemical sector thus has a challenge to reduce its climate footprint and has therefore drawn up roadmaps together with research actors (IVA, 2019). The IVA report (2019) describe how the refineries can partly change current processes to less climate-impacting, but still crude oil-based processes, and partly start refining renewable raw materials. The report also describes six partially overlapping development tracks for the Swedish chemical industry: i) Mechanical and chemical recycling of materials, ii) Transition to bio-based raw materials, iii) Transition to bio-based fuels, iv) Capture and storage of carbon dioxide (CCS), v) Recycling of carbon dioxide to new raw material (CCU), and vi) Energy efficiency.

Much faith is thus placed in future, more efficient processes and in electrification, but if a carboncontaining product is to be produced, the carbon must enter the manufacturing process from somewhere. In this study, three raw material streams are studied, all three are examples of renewable raw material streams that may satisfy this need for carbon to some extent. These streams however, largely come from industrial sectors that today are not intimately connected with the petrochemical industry, and in the interface where new collaborations need to arise there are obstacles and challenges for this collaboration to run as efficiently as possible. These two benefits are different things that are quantified in different ways, and it is also possible for a product to be circular without being climate neutral and vice-versa. This quantification can facilitate the design of policies when society wants to steer towards new value chains in collaboration with the petrochemical industry. Based on existing methods (Lönnqvist, et al., 2022), this project will also analyze the social aspects of sustainability with a focus on, for example, working conditions and the effects on the local community and population. A qualitative assessment was carried out on the effects of the new value chains compared to current practices and production methods.

A variety of studies focus on the technical prerequisites for using bio-raw materials, electro-raw materials and circular raw materials for the petrochemical industry, with the various processes required throughout the value chain. For example, development of crude oil production from forest residues (Echresh Zadeh, Abdulkhani, & Saha, 2021), lignin (Suncarbon, 2021), waste (Dyer, Nahil, & Williams, 2021), plastic waste (El-Fateh Abomohra, Sheikh, El-Naggar , & Wang, 2021) for use in oil refineries, and studies of the technical implications thereof (Pontes, Silva, Ximenes, Pinho, & Azevedo, 2021). Further studies focus on producing raw materials directly for the chemical industry based on biomass or recycled material, e.g., the project "Conversion of gasification infrastructure at Perstorp to recycled raw material and biomass" where the conditions for four possible raw material streams are evaluated (RISE ETC, 2021). In addition to the technical conditions for alternative raw materials, the techno-economic conditions and reduced emissions of greenhouse gases are also often studied (Jafri, et al. 2021). However, fewer studies focus on the organizational conditions and policy. As the new value chains require industrial sectors to start collaborating in new ways, barriers at the organizational and policy level need to be identified and

dealt with in order not to stand in the way of the transition to a circular and climate-neutral future. This study is built around the view that the petrochemical industry will need continued access to carbon atoms from some source, even when a transition to sustainable production has been completed.

This project includes three such sources: i) Residual products from the forest industry. Through thermochemical processes (pyrolysis/liquefaction, gasification), forest residues such as black liquor/lignin from the pulp industry can be converted into a bio-oil. This bio-oil is a liquid mixture primarily consisting of a complex mixture of oxygenated hydrocarbons and water (Sundberg, 2016), ii) Electrofuels. By capturing carbon dioxide from point sources and producing hydrogen gas, electro-synthetized oil can be produced in a Fischer-Tropsch synthesis process. The electro-oil is a liquid mixture primarily consisting of alkanes and alkenes with a chain length that is determined by the process conditions during the synthesis (Fagerström et. al., 2020), iii) Chemical recycling of plastic waste. Through thermochemical processes, recycled plastic can be liquefied into a recycled oil. This oil is a liquid mixture consisting of a mixture of different hydrocarbons which is determined by the recycling processes and which plastic waste goes into the processes (Henric Lassesson, 2021). The present study also assumes that existing infrastructure for refining hydrocarbon streams will continue to be useful during and after a completed conversion. Therefore, this project includes an existing refinery for the treatment of incoming streams. In the refinery, input streams will be fractionated into output streams to varying extents depending on their respective origin and content.

Certain partial streams of the respective raw material stream could be used directly in various applications (or not practically fed into a refinery) and thus bypass refining or could alternatively become high-value end products after a simpler separation process. However, this does not apply to the entire flow for any of the three raw material streams (Fagerström et. al., 2020; Henric Lassesson, 2021; Sundberg, 2016) and therefore concepts of value chains that do not need upgrading are not included in this study.

There is already ongoing cooperation in the chemical and refinery industry. Borealis' cracker is central to Stenungsund's chemical cluster and many collaborations already exist here, but there are also potential for further collaborations, for example based on opportunities for heat exchange. Other examples are that Borealis work together with Stena and Fortum to develop processes for recycling, which potentially could lead to new sources of raw material supply to Borealis (Hållbar kemi, 2022; Johanneberg Science Park, 2022; Energimyndigheten, 2022). Borealis and Stena have recently received funding by Industriklivet for a prefeasibility study of such an investment (Energimyndigheten, 2022). Another example is Perstorp's 'Project Air' that aims to produce methanol via CCU and involves many different partners and processes such as carbon capture, gasification of biomethane and residue streams, electrolysis and methanol synthesis (Project Air, 2022). Having previously being granted support from Industriklivet (Energimyndigheten, 2022) but being denied support from the EU Innovation Fund, Perstorp recently submitted an updated application to the EU Innovation Fund (Perstorp, 2022)., which has since then been granted.

The debate about circular economy and mitigating climate change has been going on for many years. In the last five years or so the chemical and refinery industries have started to realize that they must act on this to be able to continue to produce. Sites and firms located in Sweden has realized this early (c.f. e.g., (Bauer & Fuenfschilling, 2019)) but in the last couple of years also many headquarters of multinational firms have come to the same conclusions. One focus for future collaboration projects along this line (as well as the focus of the project presented in this report) is on new raw material suppliers to these industries. In the following, challenges that are perceived by the project partners towards these types of collaborations are presented. The challenges are

categorized in three categories: collaboration and coordination; financial and organizational challenges.

3 Choice of value chains

Starting from some 15 different options, five value chains were selected for further analysis within this project.

Initially, the **feedstock side** included bio-based, circular and renewable options: wood waste, lignin from the pulp industry, recycled plastic, recycled tires, renewable electricity, and captured CO₂ from wood fuel burning in CHP plants.

Then different **conversion technologies** where considered: hydrocracking, pyrolysis, gasification, fermentation, Fischer-Tropsch synthesis, alcohol-to-Jet, reverse water-gas shift reaction (rWGSR), and catalytic conversion of lignin to lignin-oil (the RenFuel process).

After conversion, a range of different **products** would be obtained. Some of them need further refining in refineries and crackers, while others may be used more or less directly to replace their fossil counterpart. Among the products are hydrocracking oil, pyrolysis oil, FT crude, methanol, ethanol. After further refining and cracking, even more products can be obtained: gasoline, diesel, waxes, jet fuel, ethylene, and propylene for the chemical industry.

In the selection process, hydrocracking was rejected due to very low technical readiness level (TRL). The alternatives using lignin as feedstock was opted out because they are analysed in depth in a parallel project at IVL. To be able to compare the analysis for different value chains, value chains leading up to the same products were finally selected for further analysis; two value chains producing FT crude and two producing methanol.

Selected value chains

Five value chains were selected. In Chapter 7, the value chains are described in detail. Value chain 1 and 3 result in production of a Fischer Tropsch (FT) crude, either from hydrogen produced with renewable electricity and carbon dioxide captured from a biofuel plant (value chain 1), or from gasification of forest residues (value chain 3). Value chain 2 and 4 result in production of methanol, based on the same raw materials as Value chain 1 and 3 respectively. Finally, Value chain 5 results in a pyrolysis oil produced from pyrolysis of plastic waste.

Value chain 1: FT crude from hydrogen and carbon dioxide.

Value chain 2: Methanol from hydrogen and carbon dioxide.

Value chain 3: FT crude from gasification of forest residues.

Value chain 4: Methanol from gasification of forest residues.

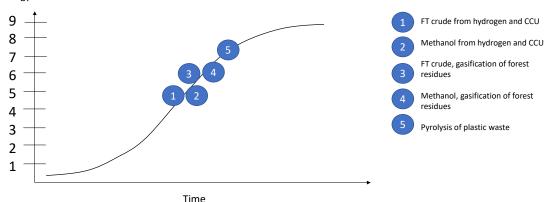
Value chain 5: Pyrolysis oil from plastic waste pyrolysis.

The three different end products (FT crude, methanol and pyrolysis oil), require different treatment to become end-user products. FT crude and pyrolysis oil need refining at a refinery, while methanol more directly can replace its fossil counterpart.

FT-crude is a mixture of mostly aliphatic hydrocarbons of varying chain length. The chain length distribution of FT-crude is determined by parameters of its production process. The mixture needs to be separated into several fractions in a refining process, typically by distillation. The fractions can then be used, depending on their properties and content, either as a fuel directly, or more likely, as a mixing component to meet fuel standards of various vehicle fuels, e.g., petrol, diesel, jet-fuel, etc.

Methanol produced through the processes described in this study, may after appropriate purification procedures, be used within the same value-chains as where its fossil counterpart is used today. Methanol is used as feedstock in the chemical industry, to produce products such as adhesives, solvents and antifreeze.

Pyrolysis oil contains a heterogeneous mixture of hydrocarbons, aliphatic, cyclic, etc. It also contains water and other impurities as well as chemically bound oxygen which needs to be removed in a chemical refinement process. This refinement process in more extensive than simply distillation and may involve both cracking and the addition of large amounts of hydrogen (IEA Bioenergy, 2020). After this processing the handling of fractions from pyrolysis oil may be similar to that of FT-crude.



Technology Readiness Level

Figure 1 Technology Readiness Level for the selected value chains shown in a S-curve for development over time. Based on the estimations of IEA Bioenergy (IEA Bioenergy, 2020).

Technology Readiness Level (TRL) describes the maturity of technologies. TRL 1 is the lowest maturity where only some basic principles for the technology have been observed. TRL 9 is the highest level of maturity, where the technology system has proven in operational environment. In Figure 1, the five selected technologies are placed on a S-curve based on which TRL they have (IEA Bioenergy, 2020). TRL 5 which value chains 1 and 2 belong to, is where the technology is validated in relevant environment, larger than lab-scale. TRL 6 is when the technology has been demonstrated in relevant environment. TRL 7 is when system prototype has been demonstrated in operational environment.

Rapport C 722 – BeKind – Cirkularitets- och klimatnytta hos en Bioelektrobaserad Kemiindustri - effekter av en omställning av petrokemins värdekedjor

4 Challenges and mitigating activities

This section focuses on challenges for a transition to value chains identified previously in this study. First, the conceptual framework used for the analysis is presented, with a particular emphasis on the category that the analysis focuses on. Secondly, we present a short review of other studies addressing barriers to a transition of the Swedish petrochemical industry. Finally, the method used in this part of the study is presented, followed by the results and analysis of this.

Challenges for a transition to a circular and climate neutral petrochemical industry have in prior studies been structured according to four categories: market barriers, technical challenges, regulatory barriers and coordination barriers (Löfgren & Rootzén, 2021). Market barriers are all related to the risks related to the market and demand of current or new products. One example is the risk that companies expose themselves to when pursuing low-CO₂ products with a higher production cost than established fossil-based products. Another example is the increased risk of exposure to exogenous market changes – such as cost of energy and raw materials – that companies face due to long planning horizons and lead times. *Technical challenges* include all challenges related to taking an innovation through all the steps of the innovation chain, including demonstrating viability in terms of both technical and commercial aspects. Regulatory barriers are challenges related to policy and regulations, which can be related both to the uncertainty caused by an unstable or unpredictable regulatory environment, but also related to differences in regulatory structures between different countries or regions. Coordination barriers are related to shifts in the sociotechnical system that are required for transitioning to sustainable products and value chains. This can be, for instance, adaptations among actors along the value chain or the availability of relevant competence within the workforce.

In this study we have a particular focus on identifying coordination barriers. Coordination has been described as one of two facets of collaboration (Gulati, Wohlgezogen, & Zhelyazkov, 2012). According to this distinction, cooperation deals with relations and aligning the interests of collaborating partners, while coordination focuses on the inter-dependencies and interorganizational interfaces and how partners will undertake their joint endeavors (Gulati, Wohlgezogen, & Zhelyazkov, 2012). While largely overlapping, the definition of coordination used by (Gulati, Wohlgezogen, & Zhelyazkov, 2012) differs slightly from the one used by (Löfgren & Rootzén, 2021) in that it gives less attention to infrastructural aspects. In this study, coordination barriers are studied less with focus on infrastructural aspects, and more focus on:

- **Collaboration and coordination** in supply chains and agreements regarding how, for instance, to specify quality of raw materials and how to share risk of investments in infrastructure.
- Financial barriers regarding how to connect both public and private financing to projects.
- **Organizational barriers** related to increasing the competence of the existing work force and securing the right expertise, but also character of ownership and requirements on payback time for investments.

A number of studies have previously identified challenges and barriers with a transition of the Swedish petrochemical industry, with some addressing all four categories of the framework by (Löfgren & Rootzén, 2021) while some give more emphasis to coordination barriers.

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(Jannasch, et al., 2020) use interviews and available literature to investigate barriers and opportunities with implementing Power-to-X technologies in the West Sweden Chemicals and Materials Cluster. While most of the barriers identified are in the technical, market and regulatory categories, they also shed light on an infrastructural coordination barrier, as they discuss the need to expand the power grid to facilitate the development of such value chains (Jannasch, et al., 2020).

As part of a task to give policy proposals for chemical recycling of plastics, (Bjerkesjö, et al., 2021) investigate barriers and potential mitigation efforts for these based on a literature study and workshops with members of the West Sweden Chemicals and Materials Cluster. Again, many of the identified barriers belong to the technical, regulatory and market categories, but they also emphasize coordination barriers, such as the issue of power supply, but also that raw material supply is hindered due to that current logistic and value chains are built up around other forms of recycling.

In a study on how the state and other actors can stimulate the climate transition for process industries, (Karltorp, Bergek, Fahnestock, Hellsmark, & Ulmanen, 2019) delve into existing literature regarding barriers for, among others, the petrochemical industry, focused on the cluster in Stenungsund. Barriers are investigated for the transition to several different value chains, including use of biobased raw materials, chemical recycling of plastics, use of CCU for methanol and olefin production and conversion of the cracker, which makes up the center of the cluster. Apart from the infrastructure-related coordination barriers of timely provision of renewable energy and raw materials, a coordination barrier is identified in creation of new networks along the value chains for biobased raw materials.

In a report for the industry and employers' organization IKEM, Material Economics investigate different value chains for transition of, among others, the petrochemical industry in Sweden (Material Economics , 2021). In the term barriers, the only coordination barrier mentioned is an infrastructure-related barrier of timely access to sufficient renewable electricity and raw materials.

In a study on multi-scalar dynamics as obstacles for industrial transition, (Bauer & Fuenfschilling, 2019) investigate the interrelations between global regimes and local sustainability initiatives by looking at one such initiative in chemical industry cluster in Stenungsund. Their main findings are that local sustainability initiatives involving multi-national companies may be hindered by the global regime in these companies in a number of dimensions. One dimension concerns the *inadequacy of networks*, where local formation of company networks might be hindered by global competition between the multi-national companies, and where partnerships with the bioresource sectors are weak. Another dimension covers *inconsistent aims and expectations* at the global and local levels, where local managers can be prepared to become frontrunners in the transition but are held back by a global rationality with a focus on incremental improvements. *Institutional contradictions* is another dimension identified as an obstacle, as sustainability in the global regime is often institutionalized as complying with regulations on emissions and workers' health and safety. Lastly, *internal competition* for resources might limit the possibilities to fund and pursue local innovative projects as priorities are set by distant headquarters.

Lastly, in a study focused on the biorefinery development in Sweden, (Mossberg, Söderholm, & Frishammar, 2021) investigate transformation challenges for incumbent actors at the network, organizational and policy levels. At the network level, which is of most relevance for the current project, they see two types of issues with actor networks for new value chains. One issue concerns actor diversity, where they argue that many actor networks suffer from at best having passive – but sometimes completely missing – participation of incumbent actors which are often deemed

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essential for commercialization of new technologies. Another issue relates to the level of collaboration in the networks, which is associated with multiple challenges for actor networks, e.g., aligning interests, coordinating the network, handling of immaterial rights, and achieving efficient role taking.

The identification of coordination barriers in this work is undertaken through a workshop with stakeholders within the relevant value chains, supplemented with individual discussions with stakeholders unable to attend the workshop. The results are processed through a synthesizing analysis in which the results are combined and evaluated. The result of the analysis is presented in the following.

Identification of challenges

Method: The first workshop focused on possible new value chains that could be developed in the sector (see section 3 for an overview of value chains). Obstacles for realizing the value chains was also discussed during the workshop and are presented below. A few project partners could not participate in the workshop, these partners were interviewed so that their view would also be reflected in the results.

Collaboration and coordination challenges

New collaborations and many actors: A challenge for the discussed value chains is that they are just new and involve new collaborations with several firms that comes with various competences, processes, culture and characteristic etc. (see Table 1). For example, the fact that the process industry run their operations continuously can be a challenge if a firm with batch production is to integrate its process into a new value chain.

Culture and firm character: Culture and other aspects that define the firm character were discussed as a possible challenge during the workshop. The firm culture could for example be formed by the nationality or sector of the firm or on what market the firm operates. As an example, a firm working with local waste collection has another perspective than a global technology provider. Also, a municipally owned company has different priorities than a publicly listed company. If two firms have not worked together before it will be challenging before they get to know each other and develop a relationship.

In Table 1, firms in a selection of value chains (Methanol or FT crude from hydrogen and carbon dioxide, Gasification and FT synthesis of plastic waste, Pyrolysis of old tires, and Black liquor to biofuels) have been characterized according to five aspects: sector, geographical market, sustainability priority, firm size and ownership. This shows that the character of the firms within the value chains varies largely in all aspects. The differences in character imply possible collaboration challenges. The size of the firm can be a challenge for collaboration, due to the imbalance in dependency towards each other. For example, if one firm is very small and should supply waste (a small quantity) and the other firm is large and should use this waste as a raw material for their process (which requires a large quantity of raw material supply). There is a concern from small firms regarding protection of their intellectual property when cooperating closely with large firms on technological development. Another example could be if the firms have different priorities in their sustainability work – e.g., maximize recycling vs producing fuel.

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Table 1 Firm characterization based on the workshop results. In the workshop focus was on the following value chains: Methanol or FT crude from hydrogen and carbon dioxide (Value chain 1 and 2 in Chapter 3, Gasification and FT synthesis of plastic waste, Pyrolysis of old tires, and Black liquor to biofuels.

Sector	Market	Most important sustainability aspect	Firm size	Ownership
Forestry	Global	Sustainable bio raw material from forestry	Large	Stock market
Energy	European	Electrification, Climate	Large, Medium	State owned, Municipality owned
Technology developer	Nordic	Sustainable bio raw material from forestry	Small	Private
Technology deliverer	Nordic, Global	Sustainable bio raw material from forestry	Small, Large	Stock market, Private
Municipality	National	Efficient resource use, Climate	Small	Municipality owned
Chemical industry	European	Climate	Large	Stock market
Refinery industry	European, Global, Sweden	Climate, Circularity	Medium, Large	Private, Family owned, State owned
Pulp and paper industry	Global, National	Efficient resource use, Climate	Small	Stock market
Transport companies	National, Nordic	Climate	Large	State owned
Recycling	National	Circularity	Small	Private

System boundaries: A challenge for collaborations in the new value chains is how to draw the system boundary (local, regional/national or global) and based on this boundary calculate impact on e.g. emissions of carbon dioxide.

Contracts: Another challenge can be contracts and how to form these between the collaborating firms. For example, for how long the contracts should be valid. The refinery industry is for example used to short contracts but to invest in new innovative processes for production of crude oil, the suppliers need to have a long-term offtake agreement.

Standards: Standards are mentioned as a difficulty that for example could concern what raw material the collaborating firms can handle in their processes. More specifically this could concern the quality of oil and refinery's ability to treat it at their site. Firms belonging to different sectors may have a challenge since different standards of quality are used.

Infrastructure and permits: To realize several of the new value chains there are needs for infrastructure investments such as the need for fossil free electricity and power grids. This is also linked to the challenge of getting permits, e.g., environmental permits. Permits could also be a challenge if the new collaborations require changes at industrial sites. Infrastructure and the need for more reliable and quick processes for permits are common challenges for many industrial transition processes in Sweden and several actions have been taken to handle them, such as governmental investigations and the national budget for handling permitting processes was increased for 2022.

End product markets, political narrative and public opinion: What markets the firms operate on can also be a challenge for the new value chains. If for example a firm operate on a market where it is difficult to distinguish or communicate between fossil and non-fossil content of the products it will be difficult to get a premium price for a new product and this can be a hinder for participating in a new collaboration. The mass balance method is often put forward to handle this communication challenge. However, some actors claim that this method will not work for them and they need a 100% biomass-based product.

Some of the participants point to political debates and public opinion and argue that these do not provide incentives for new collaborations but could rather be hindering development. An example is the strong narrative of electrification and replacement of combustions engines which could be seen as a hinder for collaborations aiming at developing biofuels. On the other hand, policy promotes production of biofuels through the reduction quota (even though the Swedish government currently plan to reduce the requirement to EU minimum level), but there is no strong incentive for production of bioplastics. However, some actors in the chemical industry do not fear there will be a lack of demand for their products since some markets, for example health care and personal care products, have a strong demand.

Financial challenges

Financial barriers do not seem to be a big concern. The participating parties believe that good ideas in the area of the new value chains will be able to finance needed capital investments. Despite the fact that the scale of the needed investments is large for many industrial actors if there is a viable business case, capital requirements and access to finance do not appear to be a challenge. However, the industrial transition is still in an early state and many investments are still to come. Governmental intervention is key for enabling these investments and the policymakers has a particular important role for risk sharing, providing leadership and stimulating market formation for example in the form of public procurement.

Organizational challenges

Global value chains: Many of the actors in the refinery and chemical industry in Sweden are part of multinational firms which means that the business case that a new collaboration represents must compete with alternative business cases at other sites globally. The prerequisites for developing these business cases and the collaboration are to a large extent determined by the conditions given by national policies. This means that a challenge for the Swedish actors is to prove that a business case and new collaboration in Sweden can outcompete a case in for example China that has a different policy landscape.

Firm culture: Participating parties mention possible challenges in general terms such as the fact that the firm culture must be forgiving and allow mistakes since mistakes are likely to happen as firms engage in new value chains.

Not core business: It is also identified that the firm core business or core competence could be a challenge depending on if the new collaboration is close to or far away from the core business or core competence. It is always challenging for firms to change core business or develop new competences.

Competence: When new processes are introduced there is a challenge of adapting and finding competence, both in terms of technical expertise and for support functions. This is a particularly large challenge when intersectoral competence is required which combine traditional areas of expertise. , In addition, lack of competence at authorities can also be a challenge since many authorities must be involved in coordinating the development of new value chains.

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Identification of mitigating activities

In a second workshop, the project partners discussed and specified activities to handle the challenges identified in the previous section. First, in smaller groups focusing on specific value chains, the challenges where concretised and it was specified in which link of the value chain each of them occurred. Then, the challenges were grouped into categories which could be handle with similar mitigating activities. For each activity it was specified which stakeholders that should be involved. Stakeholders could be both within the value chain or external. Also, a timetable was suggested pointing out which activities that are most urgent to start with, and which could be started later.

Collaboration and coordination

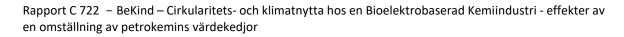
New collaboration and many actors - Example with logistics

In the context of recycling of plastic waste, there are several challenges related to logistics which require collaboration between the stakeholders. In addition, there is lack of regulation with regards to handling of waste. The collection of waste is regulated, but the following steps such as sorting, washing and size reduction are not regulated at all. Development of regulation for this is requested by the industry.

Culture and firm character - Different views on sustainability

One challenge for collaboration in future value chains is the varying priorities regarding sustainability in different sectors. One example is the forest sector which works with several sustainability issues with similarly high emphasis, e.g. biodiversity and ecosystem services, while sectors further down the value chain tend to focus mainly on greenhouse gas emissions. The workshop discussions concluded that working with multiple sustainability goals need to be spread more widely in the future. It would be advantageous if more sectors along the value chains could incorporate a more holistic sustainability view. To some extent this may come automatically, through extended collaboration and the process of learning of each other's prerequisites. However, raising awareness of the differences is important to initiate the discussions early on and avoid future conflicts.

Another example is that some sectors, especially the recycling sector, focus more on circularity, and others more on renewability. As discussed in Chapters 7 and 8, these two goals may be conflicting. Both circularity and renewability aim towards the same overarching goal, reduced climate change. However, circularity through reuse of material which reduces the demand for virgin material, and renewability through the use of raw material which are regrown relatively fast and hence do not add to emissions if the total circle of life is accounted for. But if the replacement of virgin materials is not accounted for in the case of recycled material, but only the origin of the recycled material (which often is fossil), the goals seem to be conflicting. This is illustrated in Figure 2. In order to mitigate this challenge, the suggestion is to identify the superior goals and thereby try to find a common ground.



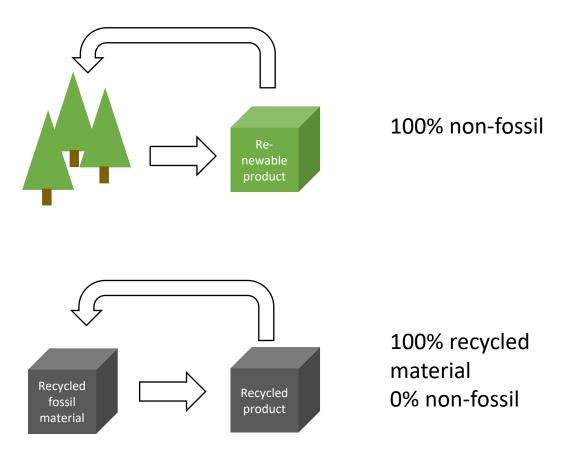


Figure 2 Renewability and recyclability are both pathways toward reduced green-house gas emissions. Renewability through the use of non-fossil resources, and recyclability through the reduced demand of virgin material. In this report they are used as two aspects of "circularity". In addition, the view on sustainability differs in different end-user segments, both in terms of different products and in different countries. This is a challenge which to some extent may be overcome with certification of origin of bio-based products which guarantees that it is from residues and/or biomass. For example, the already existing FSC certification for forest products could be expanded to also include fluids.

Standards - Quality specifications for raw materials

This issue was highlighted for several value chains. Over-specification, which makes it unnecessary difficult to reach the quality demand, is one obstacle. To mitigate this challenge, the refineries and process industries may need to review their specifications with the aim to only keep what is necessary for their specific equipment.

In value chains using recycled plastics, there are specific challenges regarding the specification of qualities and types. The viewpoints of these specifications vary between stakeholders. This needs to be solved through agreements between the stakeholders in the value chains.

Financial barriers

The industrial transition is still in an early state and many investments are still to come. Governmental intervention is key for enabling these investments and the state has a particular important role for risk sharing, providing leadership and stimulating market formation for example in the form of public procurement. The green credit guaranties introduced in the summer 2021 are mentioned (e.g. (Fossilfritt Sverige, 2022), (Maltais, Karltorp, & Tekie, 2022)) as a solution to handle the large risks involved in investments in industrial transition that can contribute to attract private capital. However, as (Fossilfritt Sverige, 2022) identifies these guaranties target investments over 500 MSEK and the Swedish Export Credit Agency targets investments under 500 MSEK with an indirect or direct link to export, but there is a gap for investments under 500 MSEK with no link to export that must be addressed.

Organizational barriers

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Global value chains - Competition within international firms

Localization of investments compete internationally in large firms. The industrial transition in Sweden, requires that investments are located here. In order to facilitate that, good conditions for industry renewal such as infrastructure and efficient permitting processes need to be provided.

Not core business - Sharing the risk of investments and long-term development

A major challenge that is identified is the difficulty to engage in long-term development projects. In large companies this may be handled by smaller teams in the outskirt of the core business. With changes in the outside world, such as economic fluctuations and world events, it may be difficult to prioritise the research and development in uncertain technologies.

One solution which may promote long-term commitment, is the forming of partnerships between several companies. Sometimes even by founding a joint venture. This may create a stable ground for the development of new technologies at the same time as it promotes the collaboration between partners needed in the future value chains.

5 Mass and energy balances

In this part of the work Fischer Tropsch crude and methanol production from different raw materials and processes were studied. The first two studied value chains, value chain 1 and 2, rely on CO₂ and H₂ as input raw materials while value chain 3 and 4 uses forest residues. The production of pyrolysis oil from plastic waste was also studied in value chain 5. The methodology used for the construction of the mass and energy balances is as follows:

- Construction and presentation of flow diagrams for the 5 different value chains identifying and defining the scope of the process units.
- Collect data describing mass and energy flows for each of the value chains
- Normalize mass flows for 1 kg product

• Normalize energy balance for 1 kg of product

In this chapter, a detail description of the value chain is done, along with the flow diagrams. In chapter 9, the overall mass and energy balances are presented and summarized in Table 10 and Table 11 as well as discussed.

FT-crude from CO₂ and H₂

The process of conversion CO₂ and H₂ into FT-crude through the Fischer Tropsch route has a TRL of 6 (Schmidt, Weindorf, Roth, Batteiger, & Riegel, 2016) but an industrial scale production plant is planned to be open in 2024 in Norway to produce 10 000 000 liters/year of e-fuels (Krohn-Fagervoll, 2022). The process described here is based on the *Bio-Electro-Jet fuel* project (Fagerström, et al., 2021) which considered and made a survey of different technologies among which the value chain as depicted in Figure 2 was selected. The scale of this study is the production of 1.7 ton/h of FT-crude with a composition of jet fuel (40%), gasoline (36%) and diesel (13%). The scope of this process for this project can be seen in Figure 2 and is the obtaining of the raw materials CO₂ and H₂, the partial conversion of CO₂ to CO and the processing of this feedstock to produce the FT-crude.

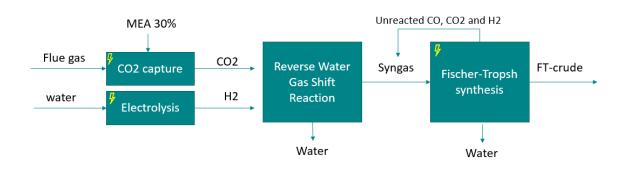


Figure 2: Flow diagram of value chain 1: production of crude FT from CO2 and H2.

The technology used for the capture of CO₂ from flue gases is a Monoethanolamine (MEA) scrubber. This uses MEA as absorbent which is introduced at a 30 wt%. This unit consists of an absorber column, and a stripper. Both the MEA solution and the flue gases enter the absorber at 40°C. The MEA rich in CO₂ leaves the absorber through the bottom and enters the stripper. The

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CO₂ is desorbed in the stripper at a temperature between 120 and 140°C and low pressure (Desideri, 2010). The MEA lean in CO₂ exits the stripper from the bottom and recirculates to the absorber. Heat recovery occurs when the lean MEA from the stripper heats up the rich MEA coming from the absorber. Part of the MEA solution is evaporated and degraded due to impurities such as SO₂, NO₂, HCl, HF, and oxygen in flue gas which means that make-up MEA solution is needed (Yang et al., 2008)(Hasan et al., 2021). The CO₂ leaves the unit at 106°C from the top of the stripper and is mixed with the H₂ flow. Electricity is also needed to run the CO₂ absorber.

The technology used for the H₂ production is Alkali electrolysis (AEL). Electricity is needed to split the water into O₂ and H₂. This electricity is produced from renewable sources.

In the reverse water gas shift (rWGS) reactor H₂ and CO₂ are heated up to 900°C. A catalyst is used to make the reaction possible. Paladium and Platinum based catalyst are selective for producing CO (Zhu et al., 2020). The rWGS reaction is an equilibrium endothermic one that produces syngas which is a mixture of H₂ and CO and in smaller amount CO₂. The goal of this step is to produce CO from CO₂ according to Equation 1 to achieve a H₂:CO ratio of about 2 (Elvers, 2008). Water is a by-product which is separated from the reactor by condensation.

$$CO_2 + H_2 \leftrightarrow H_2O + CO$$
 Eq. 1

The syngas is then compressed and heated up to 220°C before it enters the Fischer-Tropsch reactor. In this reactor H₂ and CO react with the help of a catalyst to form long hydrocarbons (FT-crude). This reaction, shown in Eq. 2 is highly exothermic, with an enthalpy of -165 KJ/molco (Fratalocchi et al., 2018). Cobalt and iron are industrially used as catalysts because of their performance and cost (Elvers, 2008) (Perego et al., 2009). Unreacted CO, CO₂ and H₂ is recirculated to the FT-reactor. The conversion of CO into FT-crude is between 60 and 90% (Luo et al., 2021).

 $(2n+1)H_2 + nCO \leftrightarrow C_nH_{(2n+2)} + nH_2O$ Eq. 2

Possible energy integration/ industrial symbiosis

This value chain has the potential to be integrated to a CHP plant. A study of this integration has been described in the *Bio-Electro-Jet fuel* project (Fagerström, et al., 2021). In this case, the fuel used in the boiler of the CHP plant was biomass and the heat produced is integrated in the FT-crude production process. This translated into saving in the heating and cooling demand (Fagerström et al., 2021).

MeOH from CO₂ and H₂

The process of conversion CO₂ and H₂ into methanol through one step reaction mechanism has a TRL of 7-8 (Irena and Methanol Institute, 2021). The largest plant is located in Iceland and produces 4 000 ton/year with plans on expansion to 100 000 ton/year by 2025 (Carbon Recycling International, 2022). The process described in this section is based on an article by Szima & Cormos, (2018). The scale of this process is the production of 12.5 ton/h of methanol. The scope of the process for this project can be seen in Figure 3 and is the obtaining of the raw materials CO₂ and H₂, its conversion to methanol and the purification of methanol.

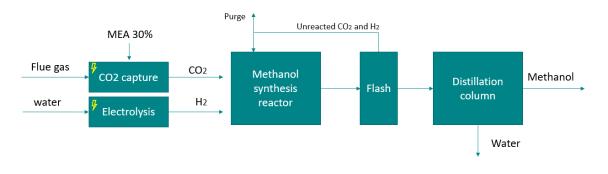


Figure 3: Flow diagram of value chain 2: production of methanol from CO2 and H2.

The CO₂ capture unit was not included in the Szima & Cormos study and for this reason data from value chain 1 was taken. The H₂ production is done in the same way as in value chain 1. H₂ and CO₂ are fed in the reactor at a pressure of 8 MPa and temperature of 210°C. The methanol synthesis reactor uses Cu/ZnO/Al₂O₃ as catalyst. The reaction that occurs in the reactor is shown in Equation 3. This is a highly exothermic reaction, having an enthalpy of -49.5 K//mol (Guil-López et al., 2019). The CO₂ overall conversion is of 97% (Szima & Cormos, 2018).

$$CO_2 + 3H_2 \rightarrow CH_3OH + H_2O$$
 Eq. 3

Liquid methanol, water and unreacted gases leave the reactor at 30°C and same pressure. The unreacted gases are separated from the liquids in the flash vessel and recirculate to enter the reactor again. The methanol and water are depressurized to almost atmospheric pressure and heated up to 80°C to enter a distillation column and be separated. The final methanol has a purity of 99%.

Possible energy integration/ industrial symbiosis

The process described in this paper was not integrated with other industry. Nevertheless, it was optimized with energy recovery from gas and steam turbines as well as the use of an organic Rankine cycle (ORC). Purge hot gases are used to produce both electricity and steam (energy recovery). The heat released by the methanol reaction is used to produce steam which is later used to produce electricity. An Organic Rankine Cycle (ORC) is also introduced to reduce the energy consumption. The electricity produced by the gas and steam turbines as well as the ORC is enough to cover the compressor units need in the process but not to cover the demand of the electrolyser.

FT-crude from gasification of forest residues

The process of converting forest residue to FT-crude through gasification, followed by FT synthesis has a TRL of 6-7 (Hrbek, 2021). The largest production plant is in France and produces 8 000 ton/year from forest residues since 2021. In the USA, a bigger plant with a production of 44 000 ton/year is under construction (Hrbek, 2021). The process described in this section is based on the paper by Holmgren et al., (2016). The scale of this process is the production of 16.1 ton/h of FT-crude with a composition of diesel (73%) and gasoline (27%). The scope of this process for this project can be seen in Figure 4 and is the preparation of raw materials forest residues and O₂ (drying and air separation), obtaining of syngas from gasification of forest residue, syngas cleaning and processing of syngas to produce FT-crude.

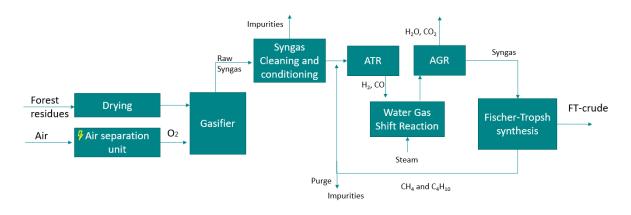


Figure 4: Flow diagram of value chain 3: production of FT-crude from gasification of forest residues

The forest residue is first chipped and dried to 15 wt-% moisture content before the gasification. Biomass moisture content is typically between 5 and 35% (Choudhury, Chakma, & Moholkar, 2015). The forest residues described in this process had 50% moisture content. The dry of the forest residues consumes approximately 2750 kJ/kg water evaporated (Isaksson et al., 2012). The dried forest residue is thereafter converted into raw syngas through gasification. Biomass gasification is usually performed at lower temperatures that coal gasification. Gasification can be performed at high or low pressures. High pressures favour the formation of methane but also reduces the cost of downstream compressions. When pressure is low the formation of methane and tars (impurities) is lower but the H₂:CO ratio is less than 1 (Bain, 1992) which will mean that a reverse water gas shift reactor is needed to adjust the ratio until about 2. The gasification described in this process is done using a pressurized oxygen- and steamblown circulating fluidized bed (CFB) operating at 25 bar and 850°C. The use of oxygen instead of air has the advantage of a cleaner raw syngas without nitrogen. An air separation unit (ASU) is required which consumes 300 kWh/ton of O₂. Oxygen is feed in a rate of 0.25 to 0.35 ton O₂/ton Biomass.

A bubbling fluidized bed (BFB), operating at 850°C is then used for catalytic cracking of tars and hydrocarbons formed during the gasification. The product of the cracking process is carbon monoxide and hydrogen, which leaves the cracker at 670°C. In order to avoid poisoning of the catalyst used in the FT synthesis, particulates and impurities are removed from the product gas through a low temperature wet gas cleaning step (Hamelinck and Faaij, 2002). The cleaning consists of a cyclone to remove solid particles; scrubbers to remove alkali, as well as sulphuric and nitrogenous compounds; and bag filters. The gas is cooled down to 40°C in the scrubbers before exiting the cleaning step.

After cleaning and conditioning of the syngas, the relatively high content of methane is reformed into CO and H₂ by the utilization of an oxygen-blown autothermal reformer (ATR) according to Equation 4. The resulting outlet stream has a temperature of 1000°C. The H₂ to CO ratio is thereafter adjusted by utilizing the WGS reaction. Prior to the FT synthesis and to avoid catalyst poisoning, CO₂ is removed by the use of an acid gas removal unit (AGR). This unit uses methanol as absorbent which is regenerated and recirculated within the unit (Yakub Mohammed et al., 2014).

$$CH_4 + H_2O \leftrightarrow CO + 3H_2$$
 Eq. 4

FT synthesis occurs in a slurry-phase reactor (SPR) at 23 bar and 210°C in the presence of a Co catalyst. The reaction is an exothermic type of reaction and is shown in Equation 2. The CO conversion is 90% per pass. Unreacted gases from the SPR unit are recycled back to the ATR in

order to crack the methane and butane compounds that has been produced during the FT synthesis. The off-gases from the synthesis process are combusted in an existing boiler.

Possible energy integration/ industrial symbiosis

The process described by (Holmgren et al., 2016) is integrated with an industrial cluster. A big part of the heat produced by the gasification is used to cover the demand of a refinery in the cluster. A steam cycle is used to recover the energy produced by the process and to be used in the process. The study does not specify if the heat demand needed for the drying of the forest residues is done within the process and/or the cluster and therefore, this demand is added to the energy balances.

MeOH from gasification of forest residues

The process of conversion forest residues to syngas by gasification and the later synthesis of methanol from syngas has a TRL of 6-7 (Hrbek, 2021). The largest production plant is located in Canada and produces 1000 ton/year from wood waste and municipal solid waste since 2009. The process described in this section is based on the paper by Holmgren et al., (2016). The scale of this process is the production of 11 ton/h of methanol. The scope of this process for this project is the preparation of raw materials forest residues and O₂ (drying and air separation), the thermal conversion of the forest residues to syngas in the gasifier, the cleaning of the raw syngas, the conversion of syngas to methanol and finally the purification of methanol.

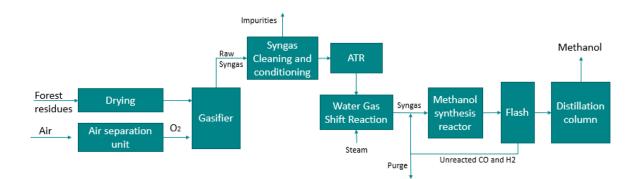


Figure 5: Flow diagram of value chain 4: production of methanol from gasification of forest residues

This process is very similar to the previous one. The difference in the cleaning step is that for the methanol synthesis, no AGR is needed since CO₂ will be consumed in the synthesis reaction.

The methanol synthesis reactor is a slurry bubble column where methanol can be produced from both CO and CO₂ according to the two equilibrium reactions shown in Equation 5 and 6. This is a catalytic type of reaction using Cu/Zn/Al as catalyst, at 90 bar and 240°C. The conversion of CO in the reactor is 75%. Unreacted CO and H₂ is recirculated back to the synthesis reactor. Part of the gases that recirculate are purged and combusted for energy production. The product from the synthesis reactor is a mix of liquid and gases that are separated in 2 flash vessels. Afterwards, the methanol is purified in 2 distillation columns. The final product is liquid methanol with a purity of 99.7% The wet biomass (feedstock) to fuel (methanol) efficiency is about 51%.

$CO + 2 H_2 \leftrightarrow CH_3OH$	Eq. 5
$CO_2 + 3H_2 \leftrightarrow CH_3OH + H_2O$	Eq. 6

Possible energy integration/ industrial symbiosis

In a standalone case, the heat produced in the methanol synthesis reactor could be used to dry the wood. The purged gases are also used to produce energy in a steam boiler, which will then run a steam turbine to produce electricity. Integration with an industrial cluster was investigated by (Holmgren et al., 2014). The results in terms of energy are a supply of steam to the cluster.

Pyrolysis oil from the pyrolysis of plastic

The process of thermally decomposing mixed plastic waste into pyrolysis gas and oil, through pyrolysis, is based on the paper by Williams & Williams, (1997). The scale of this process is the production of 0.75kg of pyrolysis oil (lab scale). This paper was chosen due to availability of data for the mass balances, even though the publication year is old. The scope of this process for this project can be seen in Figure 6 and is the obtaining of pyrolysis oil from pyrolysis of mixed plastic waste.

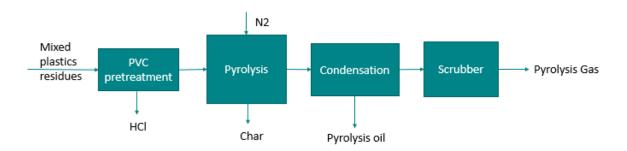


Figure 6: Flow diagram of value chain 3: production of pyrolysis oil from the pyrolysis of plastic

The inlet of this process is a mixture of plastic including low density polyethylene (LDPE) (31.25%) high density polyethylene (HDPE) (31.25%) polypropylene (PP) (7.29%) polystyrene (PS) (13.5%) polyvinyl chloride (PVC) (11.46%) and polyethylene terephthalate (PET) (5.21%), which aim to represent the plastic fraction of municipal waste in Europe. This mixture should first go through a pretreatment where chlorine content coming from PVC is reduced. This step is of importance since this can cause corrosion in the equipment and the contamination of the pyrolysis oil with organochloride compounds (Torres et al., 2020). The pretreatment can be done by the use of a extruder at a temperature where the PVC can decompose and form hydrogen chloride (HCl) gas. This is above 300°C (Wenning, 1993). This gas can be converted to hydrochloric acid (HCl_(aq)) and sold as a by-product. The use of a gas-liquid fluidized bed has also been proposed for the chlorine removal (Yuan et al., 2014). If there is still HCl in the gas, this can be removed by a dry scrubber (Torres et al., 2020).

Pyrolysis can be either a thermal or catalytic decomposition and is performed at temperatures between 300 – 900°C in an oxygen free environment. The temperature used in this concrete study from Williams & Williams (1997) was 700°C. During pyrolysis of plastic waste, the polymers are broken down into a mix of different, smaller, hydrocarbons. The pyrolysis product consists of

condensable vapors (pyrolysis oil) and a non-condensable fraction (pyrolysis gas). N2 is feed to the reactor to facilitate the move of the gases to the condenser (Eze et al., 2021).

The main difference between thermal and catalytic pyrolysis is that the presence of a catalyst lowers the energy requirements and affects the composition of the product. Commonly used catalysts are fluid catalytic cracking (FCC), silica alumina and zeolites (Eze et al., 2021). Out of these catalysts the zeolites tend to give more gaseous product. A higher operating temperature increases the yield of gaseous products and as a result the catalyst has less significant effect on the liquid yield at higher operating temperatures. To obtain a high yield of pyrolysis oil the pyrolysis should preferably occur at low temperatures in the presence of a catalyst. Nevertheless, the process described in this study was a thermal pyrolysis one and the pyrolysis oil had higher yield than the gas (75% in comparison to 9.7%).

To get the condensable oil, a quick cooling is needed. The temperatures can be under 0°C and a cooling agent would be needed. The non-condensable gases pass through a scrubber which will remove pollutants such as ammonia, hydrogen cyanide and hydrogen chloride (Wenning, 1993). The final product pyrolysis oil has a heating value between 41 and 44 MJ/kg (Miandad et al., 2019).

Possible energy integration/ industrial symbiosis

The process described in this section was done at a lab scale, where the reactor was heated by an electrically heated ring furnace. In a larger scale the energy required by the process of pyrolysis of plastic could be covered by some byproducts of the same process. Pyrolysis gas has a heating value of approximately 45 MJ/kg and can be combusted to run the pyrolysis reactor (Williams & Williams, 1997).

6 Circularity assessment

In this chapter, the circularity benefits of the five different fuel productions are evaluated. The evaluation is done by adopting the method developed by (Lönnqvist, et al., 2022),. While circular economy may have different definitions, e.g. waste and pollution minimization or maintain use of product and material, Lönnqvist et al. tackle the circularity part of the concept by its literal meaning. Namely that something being circular should be based on renewable inputs or use secondary resources. Hence, the adopted circularity evaluation method is based on two key indicators: renewability and recyclability of the material and energy inputs and outputs of the production systems (Lönnqvist, et al., 2022). Notice that the term recyclability is used in the adopted method. Usually, the term refers to the capability of a material to be recycled or reused in another process after it has been used once. In (Lönnqvist, et al., 2022), recyclability is referred to whether the material and energy input is originated from secondary sources or not. However, this recyclability indicator can be misinterpreted as the ability of the final product to be reused or recycled in the next product system. To avoid a potential misunderstanding, this report will use the term "recycled content" instead to recyclability throughout the report.

Renewability is the second indicator used in the method. It is defined as whether the material and energy come from renewable source or not (Lönnqvist, et al., 2022). In this report, the calculation of the renewability indicator was based on the renewable fraction that the material and energy input contain.

A schematic method is shown in Figure 7 below.

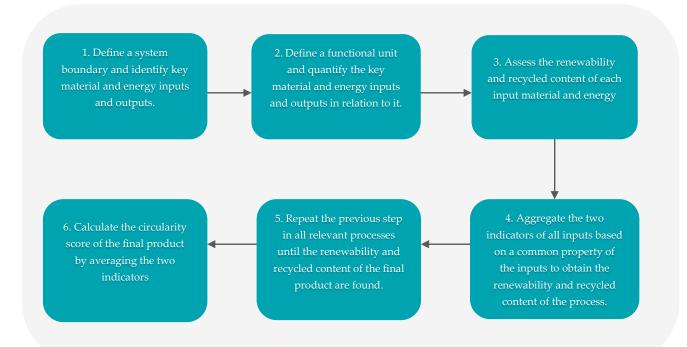


Figure 7. Description of the circularity evaluation method used in this study.

Initially, (Lönnqvist, et al., 2022) developed this circularity evaluation method to assess the circularity of transportation fuels. This means that it does not take into account the afterlife of the

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product. Namely, the possibility that the product can be recycled or reused several times. This method has not been widely used as it has recently been developed. Despite having another approach to assess the circularity, this method was chosen and applied in this project. The choice of the method was justified as all value chains uses waste as their main feedstock. Normally, circularity indicators of a process can be calculated in relation to the virgin raw material or primary energy consumption. Some examples of these indicators are resource productivity, percentage of non-virgin material used, percentage of renewable energy consumption (Gençer, 2022). However, as no virgin feedstock are considered in the value chain, it would be a challenge to use these common measurements.

In addition, for some products, it can be difficult to determine if the product can be recycled in many cycles or if it is recyclable at all. Hence, it is considered an advantage to be able to assess the circularity of a product without the end-of-life information.

Scope of the value chains

The five chosen fuel production value chains are two FT-crudes and two methanol, which are produced through biogenic CO₂ and H₂ and through gasification of forest residue, as well as pyrolysis oil from pyrolysis of plastics. The first step of evaluating the circularity of these fuels is to define a system boundary and identify key material and energy inputs and outputs. The system boundary for each value chain looks differently according to the nature of the feedstock of each value chain and the level of detail of the mass and energy balances that are available. Downstream processes of the product such as distribution, use phase and the end-of-life are excluded in the assessment for the sake of comparability between the value chains.

For the FT crude and methanol that are produced via CO₂ and H₂, the system boundary starts at the CO₂ capture process and the electrolysis of water to produce H₂. For the FT-crudes and methanol produced via gasification of forest residue, the system is modelled as a black box where forest residue and oxygen are fed to the production plant. Hence no upstream processes are included.

Similarly for the pyrolysis oil, the system boundary is set gate-to-gate which means that the system only contains the production process itself. The system boundaries of the five value chains are illustrated in Figure 8, 9 and 10. Key material and energy inputs and outputs are identified according to the mass and energy balance in Chapter 7.

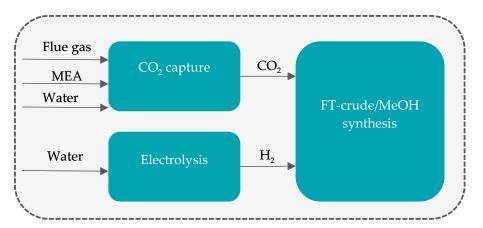
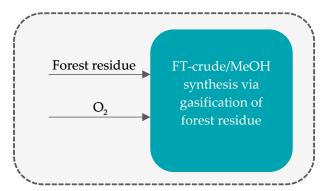


Figure 8. The system boundary of FT-crude and methanol produced from CO2 and H2



C

Figure 9. System boundary of FT-crude and methanol produced from forest residue

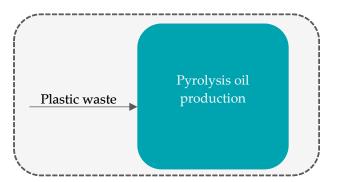


Figure 10. System boundary of pyrolysis oil from plastic waste

The second step is to quantify the inputs and outputs of the relevant processes in each value chain and define a functional unit. This input and output data for each value chain are already obtained from the mass and energy balance in Chapter 7. The functional unit used in this calculation is defined as 1 kg of fuel. It is noteworthy that energy recovery or energy integration which is normally utilized in a chemical process are not included in the calculation as they are not considered as inputs nor outputs.

Once the key inputs and outputs are quantified, their renewability and recycled content need to be assessed. For inputs that come from renewable source such as forest residue, water and oxygen, the renewability is set to 100%. The recycled content is assessed based on the secondary nature of the material and energy. For example, forest residue and plastic waste, they are considered as secondary materials which can be reused or recycled. Thus, it has 100% recycled content. Oxygen and water are considered as primary material and therefore they have 0% recycled content. If it is known that the water has been used in another process before it goes to the treatment plant, then the recycled content of this water would have been 100%. However, in this calculation, none of the water and oxygen or other similar material are assumed to be of secondary nature.

The fuel production process does require electricity. In this study, the Swedish electricity production mix in 2020 (IEA, 2020) was used to evaluate its renewability and recycled content. The calculation was based on the share of energy sources in the electricity generation mix which have different renewability and recycled content.

From the calculation, the renewability of the electricity is 66.7% and the recycled content is calculated to be 5.1%. The recycled content in the Swedish electricity productions refers to non-

renewable and renewable waste as well as household waste. Heat demand in form of steam is assumed to come from heat waste from biomass, which gives it 100% renewability and 100% recycled content. In addition, it is difficult to determine the energy source for the cooling demand. Thus, it is assumed that the cooling demand was assumed to be delivered by heat pumps.

The next step is to aggregate the renewability and recycled content of all the inputs in each process to obtain the value of the two indicators for the output in each respective process. To be able to do this, a common property between material and energy is needed. In this study, economic value (cost) of the inputs is used to weighted aggregate the two indicators. This means that inputs that have a bigger share of the total cost of the production (cost of material and energy inputs) will have bigger influence on the resulting aggregated indicators.

The economic value was chosen as a basis for the weighted aggregation because it can reflect the market situation (scarcity) of the inputs, and it is also one of the common properties between the material and energy in which data can be obtained easily. The possibility to separate the circularity assessment of the material and energy flows to avoid aggregating physical (material) andnon-physical property (energy) has been discussed in the project. However, this would mean that the assessment will have two circularity scores, one that indicates the circularity benefit of material and one for the energy. As it is not clear whether the energy is more valuable than the material or the other way around, the result from this approach can be difficult to use for the decision makers.

The price of different inputs used in the study and for all five value chains are shown in Table 2.

Material/Flow	Aaterial/Flow Price		Unit Comment	
Flue gas	0.59	SEK/kg	Cost of CO2 capture as a way of getting rid of the from flue gases	(Raksajati, Ho, & Wiley, 2013)
MEA	13.64	SEK/kg	Based on Belgian data from 2007 but assumed to represent current European market conditions	(Intratec, u.d.)
Electricity	2.64	SEK/kWh	Swedish electricity price, second half of 2021 for non-consumers.	(Eurostat, 2021)
Steam (natural gas)	0.17	SEK/kWh	Total price incl. taxes	(SCB, 2021)
Steam (biomass)	0.22	SEK/kWh	Based on average of all biomass fuel used by industries	(Vinterbäck, 2021)
Water	0.036	SEK/kg	Average price	(Privata Affärer, 2009)
H2	54.13	SEK/kg	Average price	(Kayfeci, Keçebaş, & Bayat, 2019)
Forest residue	0.76	SEK/kg	Average price of wood chips.	(Vinterbäck, 2021)

Table 2: Prices of inputs used as a basis for aggregating renewability and recycled content indicators.

For value chain that contains several stages or processes, the evaluation of the renewability and recycled content of the inputs are repeated in the next step until the indicators for the final output in the defined system boundary are found. When the renewability and recycled content of the final product are found, the last step is to calculate the circularity score of the product. This is done by weighting the renewability and recycled content indicator of the final product. In this study, both indicators are considered to be equally important. Thus, the circularity score was calculated by using the average of both indicators. The calculation of the circularity of each value chain is shown below.

FT-crude from CO₂ and H₂

The evaluation of the circularity benefit of the FT-crude from CO_2 and H_2 is shown in Table 3. The inputs and outputs are based on data used in Chapter 7.1. The renewability of the MEA is calculated based on a generic data of a production of MEA found in Ecoinvent database (version 3.6) (Ecoinvent , 2022). The indicator is calculated from the share of the total use of renewable primary energy resource of the total use of primary energy resource of the production of MEA. In the electrolysis process, O_2 is co-produced with H_2 . The circularity score of the FT-crude from CO_2 and H_2 in this study is calculated to be 77.7%.

CO ₂ capture								
Material Input	Amount [kg]	Renewable fraction	Recycled fraction	% of total cost	Cost [SEK]	Price [SEK]/kg		
Flue gas 58.14		100%	100%	77,9%	34.33	0.59		
MEA	0.02	3%	0%	0.6%	0.26	13.64		
Water	1.68	100%	0%	0.1%	0.06	0.04		
Energy Input	Amount [kWh]	Renewable fraction	Recycled fraction	% of total cost	Cost [SEK]	Price [SEK]/kWh		
Electricity	2.24	66.6%	5.1%	13.4%	5.91	2.64		
Steam	10.68	100%	100%	5.3%	2.35	0.22		
Cooling demand	0.43	66.6%	5.1%	2.6%	1.13	2.64		
Output	Amount [kg]	Renewable fraction	Recycled fraction			Total cost [SEK]		
CO ₂ excl. cooling	4.13	94.1%	84.1%			44.05		
Electrolysis								
Material Input	Amount [kg]	Renewable fraction	Recycled fraction	% of total cost	Cost [SEK]	Price [SEK]/kg		
water	5.20	100%	0%	0.2%	0.19	0.036		
Energy Input	Amount [kWh]	Renewable fraction	Recycled fraction	% of total cost	Cost [SEK]	Price [SEK]/kWh		
Electricity	29.36	66.6%	5.1%	99.0%	77.55	2.64		
Cooling demand	2.20	66.6%	5.1%	0.7%	0.57	0.26		
Output	Amount	Renewable fraction	Recycled fraction			Total cost [SEK]		
H ₂	0.58	66.7%	5.1%			78.31		
02	4.62	66.7%	5.1%					
rWGSR								
Material Input	Amount [kg]	Renewable fraction	Recycled fraction	% of total cost	Cost [SEK]	Price [SEK]/kg		
CO ₂	4.13	94.1%	84.1%	77.8%	181.97	44.05		
H ₂	0.58	66.7%	5.1%	19.3%	45.23	78.31		
Energy Input	Amount [kWh]	Renewable fraction	Recycled fraction	% of total cost	Cost [SEK]	Price [SEK]/kWh		
Steam	9.1	100%	100%	0.9%	2.01	0.22		
Cooling demand	1.8	66.6%	5.1%	2.0%	4.73	2.64		
Output	Amount [kg]	Renewable fraction	Recycled fraction			Total cost [SEK]		
Syngas	10.65	88.3%	67.4%			233.93		
FT synthesis								
Material Input	Amount [kg]	Renewable fraction	Recycled fraction	% of total cost	Cost [SEK]	Price[SEK]/kg		

Table 3. The circularity evaluation of FT-crude via CO2 and H2

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Syngas	10.65	88.3%	67.4%	99.62%	2491.35	233.93	
Energy Input	Amount [kWh]	Renewable fraction	Recycled fraction	% of total cost	Cost [SEK]	Price[SEK]/kWh	
Electricity	2.27	66.6%	5.1%	0.24%	5.99	2.642	
Steam	1.19	100%	100%	0.01%	0.26	0.22	
Cooling demand	1.28	66.6%	5.1%	0.1%	3.37	2.642	
Output	Amount [kg]	Renewable fraction	Recycled fraction			Total cost [SEK]	
FT-Crude	1.000	88.2%	67.1%				
Circularity benefit of the value chain							
Final product	Amount [kg]	Renewable fraction	Recycled fraction	Circularity score			
FT-crude	1	88.2%	67.1%				

Methanol from CO_2 and H_2

The evaluation of the circularity of the methanol from CO_2 and H_2 is shown in Table 4. The inputs and outputs are based on data used in Chapter 7.2. The circularity score of the methanol from CO_2 and H_2 in this study is calculated to be 78.2%.

CO ₂ capture							
Material Input	Amount [kg]	Renewable fraction	Recycled fraction	% of total cost	Cost [SEK]	Price [SEK]/kg	
Flue gas	22.87	100%	100%	81.9%	13.50		0.59
MEA	0.007	3.0%	0%	0.6%	0.10		13.64
Water	0.66	100%	0%	0.1%	0.02		0.036
Energy Input	Amount [kWh	Renewable fraction	Recycled fraction	% of total cost	Cost [SEK]	Price [SEK]/kWh	
Electricity	0.76	66.6%	5.1%	12.3%	2.02		2.64
Steam	2.00	100%	100%	2.7%	0.44		0.22
Cooling demand	0.15	66.6%	5.1%	2.4%	0.39		2.64
Output	Amount [kg]	Renewable fraction	Recycled fraction			Total cost [SEK]	
CO ₂	1.55	94.5%	85.4%				16.47
Electrolysis							
Material Input	Amount [kg]	Renewable fraction	Recycled fraction	% of total cost	Cost [SEK]	Price [SEK]/kg	
water	1.80	100%	0%	0.2%	0.06		0.036
Energy Input	Amount [kWh	Renewable fraction	Recycled fraction	% of total cost	Cost [SEK]	Price [SEK]/kWh	
Electricity	10.40	66.6%	5.1%	93.2%	27.47		2.64
Cooling demand	0.74	66.6%	5.1%	6.6%	1.95		2.64
Output	Amount [kg]	Renewable fraction	Recycled fraction			Total cost [SEK]	
H ₂	0.19	66.7%	5.1%				29.49

Table 4. The circularity evaluation of methanol from CO2 and H2

02	1.55	66.7%	5.1%				
MeOH synthes	is						
Material Input	Amount [kg]	Renewable fraction	Recycled fraction	% of total cost	Cost [SEK]	Price [SEK]/kWh	
CO ₂	1.55	94.5%	85.4%	78.2%	25.54		16.47
H ₂	0.19	66.7%	5.1%	1 7.2%	5.60		29.49
Energy Input	Amount [kWh	Renewable fraction	Recycled fraction	% of total cost	Cost [SEK]	Price [SEK]/kWh	
Cooling demand	0.57	66.6%	5.1%	4.6%	1.50		2.64
Output	Amount [kg]	Renewable fraction	Recycled fraction			Total cost [SEK]	
Methanol	1.55	88.5%	67.9%				32.63
Circularity benefit of the value chain							
Final product	Amount [kg]	Renewable fraction	Recycled fraction	Circularity score			
Methanol	1	88.5%	67.9%		7	8.2%	

FT-crude from forest residue

The evaluation of the circularity of the FT-crude from gasification of forest residue is shown in Table 5. The inputs and outputs are based on data used in Chapter 7.3. The circularity score of the FT-crude from forest residue in this study is calculated to be 79.2%.

FT synthe	esis from	biomass ga	sification					
Material Input	Amount [kg]	Renewable fraction	Recycled fraction	% of total cost	Cost [SEK]	Price [SEK]/kg		
Wet biomass	11.09	100%	100%	61.2%	8.42	0.76		
O ₂	1.94	100%	0%	3.8%	0.53	0.27		
Energy Input	Amount [kWh]	Renewable fraction	Recycled fraction	% of total cost	Cost [SEK]	Price [SEK]/kWh		
Electricity	1.53	66.6%	5.1%	29.4%	4.05	2.64		
Heat	3.49	100%	100%	5.6%	0.77	0.22		
Output	Amount [kg]	Renewable fraction	Recycled fraction			Total cost [SEK]		
FT-crude	1	90.2%	68.2%			13.77		
Circularity benefit of the value chain								
Final product	Amount [kg]	Renewable fraction	Recycled fraction	Circularity score				
FT-crude	1	90.2%	68.2%		79.2%			

Methanol from forest residue

The evaluation of the circularity of the methanol from gasification of forest residue is shown in Table 6. The inputs and outputs are based on data used in Chapter 7.4. The circularity score of the methanol from forest residue in this study is calculated to be 82.8%.

Material Input	Amount [kg]	Renewable fraction	Recycled fraction	% of total cost	Cost [SEK]	Price [SEK]/kg	
Wet biomass	16.23	100%	100%	72.2%	12.32		0.76
O ₂	2.84	100%	0%	4.5%	0.77		0.27
Energy Input	Amount [kWh]	Renewable fraction	Recycled fraction	% of total cost	Cost [SEK]	Price [SEK]/kWh	
Electricity	0.51	66.6%	5.1%	7.9%	1.34		2.64
Cooling demand	1.00	66.6%	5.1%	15.5%	2.6		2.64
Output	Amount [kg]	Renewable fraction	Recycled fraction			Total cost [SEK]	
Methanol	1.00	92.2%	73.3%				17.08
Circularity benefit of the value chain							
Final product	Amount [kg]	Renewable fraction	Recycled fraction	Circularity score			
Methanol	1	92.2%	73.3%	82.8%			

Table 6. The circularity evaluation of methanol from gasification of forest residue

Pyrolysis oil from plastic waste

The evaluation of the circularity of the pyrolysis oil from plastic waste is shown in Table 7. The inputs and outputs are based on data used in Chapter 7.5. As there is no reliable statistic on the share of biobased plastic waste on the Swedish market, the renewability indicator of the plastic waste is estimated to be between 1-2% based on an expert judgement by Rickard Jansson, Swedish Plastic Recycling. The energy demand in the pyrolysis process normally come from an internal combustion of pyrolysis gas which is the co-product of the process. Hence, the energy inputs are not shown in the calculation in Table 7. The circularity score of the pyrolysis from plastic waste in this study is calculated to be 51%.

Pyrolysis oil synthesis							
Material Input	Amount [kg]	Renewable fraction	Recycled fraction	% of total cost	Cost [SEK]	Price [SEK]/kg	
Plastic waste	1.33	2%	100%	100.0%	4.34	3.26	
Output	Amount [kg]	Renewable fraction	Recycled fraction			Total cost [SEK]	
Pyrolysis oil	1.00	2%	100%			4.34	
Char	0.04	2%	100%				
Pyrolysis gas	0.13	2%	100%				
System circularity							
Final product	Amount [kg]	Renewable fraction	Recycled fraction	C	ircularity score		

Table 7. The circularity evaluation of pyrolysis oil from pyrolysis of plastic waste



Pyrolysis oil	1	2%	100%	51.0%
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Result

The summary of the result from the evaluation of circularity benefits of the five fuel product value chains is shown in Table 8. The result shows that the production of methanol and FT-crude from the gasification of forest residues have higher circularity score than those produced from CO₂ and H₂. The circularity score of the FT-crude from forest residue is 79.2% while it is 77.7% for FT-crude from CO₂ and H₂. The circularity score for the methanol from forest residue is 82.8% while for the electrofuel synthesis (CO₂+H₂) route, the score is 78.2%.

Value chain	Renewability	Recycled content	Circularity score
FT crude from CO ₂ +H ₂	88.2%	67.1%	77.7%
FT crude from forest residue	90.2%	68.2%	79.2%
MeOH from CO ₂ + H ₂	88.5%	67.9%	78.2%
MeOH from forest residue	92.2%	73.3%	82.8%
Pyrolysis oil	1-2%	100%	51%

Table 8. Summary of the evaluation of the circularity benefits of five different value chains

The gasification of forest residue value chain has higher circularity score because their feedstock, which are biomass and oxygen, have 100% renewability as they enter the production process. Thus, the upstream processes of producing these feedstocks are not taken into account. On the contrary, for the electrofuel value chain, the process of capturing CO₂ from flue gas and the electrolysis of water are considered. This leads to the feedstock of the electrofuel having a lower renewability when they enter the production process compared to the feedstock for the gasification process. Similarly, the recycled content of the inputs of the gasification process are slightly higher than for the electrofuel value chain. This results in a higher circularity overall for the fuel producing from forest residue.

For the pyrolysis oil from plastic waste, the circularity score is 51%. The pyrolysis oil has a low circularity since the only contributing input is plastic waste which has a very low renewable fraction (1-2%).

Comparing to FT-crude and methanol regardless the production pathways (CO₂+H₂ or gasification of forest residue), the result shows that methanol production has higher circularity than FT-crude.

Sensitivity analysis

Since the electrofuel value chainrequired a significantly higher electricity demand, it is interesting to see if the overall result would change if a 100% renewable electricity is used in all the processed.

Here it is assumed that the price of both type of electricity is the same. The result is shown in Table 9.

 Table 9. A comparison of the circularity when the Swedish electricity is 100% renewable compared to the reference cases

Production value chain	Circularity (reference)	Circularity (100% renewable electricity)
FT-crude (CO ₂ +H ₂)	77.7%	83.3%
FT (forest residue)	79.2%	84.1%
MeOH (CO ₂ +H ₂)	78.2%	83.7%
MeOH (Forest residue)	82.8%	86.7%
Pyrolys of plastic waste	51.0%	51.0%

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Table 9 shows that the circularity score in all cases is increased. However, the overall conclusion does not change. The gasification of forest residue value chain has higher circularity benefit than the electrofuel value chain.

The price of the input material and energy can also affect the result. In this case, the price of electricity and flue gas are chosen as the inputs of interest. Sensitivity analyses are done to investigate the effect of the prices on the circularity of the five value chains. The price of electricity used in the calculation is 2.64 SEK/kWh which is the price of electricity in the second half of 2021 in Sweden. However, due to the current situation where there is a shortage of energy in Europe and a low supply capacity in Southern Sweden, the price of electricity can be expected to be higher than assumed here in the coming years. To capture the effects of varying electricity prices the electricity price is doubled, tripled and halved in the sensitivity analysis.

The price of flue gas was assumed to be equal to the cost of getting rid of the flue gas in the CO₂ capture process. The cost was taken from (Raksajati, Ho, & Wiley, 2013) where the cost range was estimated to between 62-80 USD/t CO₂, which correspond to 516-665 SEK/t CO₂. According to Raksajati et al. the most likely cost is 71 USD/t CO₂, which correspond to 590 SEK/t. In the sensitivity analysis, the lowest price, highest price, mostly likely price and when the price increased significantly e.g. up to 900 SEK/t CO₂ are tested. The results from the two sensitivity analyses are shown in Figure 11 and 12. Pyrolysis oil are excluded from the analyses since the value chain does not have electricity and flue gas as its key material inputs.

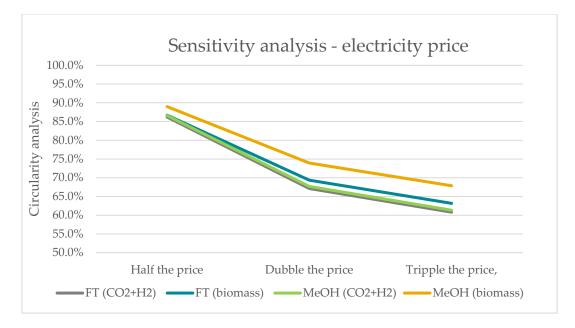


Figure 11. Sensitivity analysis of the circularity score of different value chains to the electricity price

Figure 11 shows that the circularity score decreased as the price increase. This is expected as the aggregation method of the renewability and recycled content indicator were based on prices. The higher the price of an input, the more it weighs on the final circularity score. Since the Swedish electricity grid contains a low share of recycled content and 66.6% renewability, it gives a negative impact when the electricity has more and more influence on the result.

Figure 6 also shows that the energy intensive synthesis of electrofuel is the most sensitive to electricity price and the production of methanol from forest residue is the least sensitive. It also shows that the circularity benefit of the gasification of forest residue value chain is still higher than the electrofuel value chain.

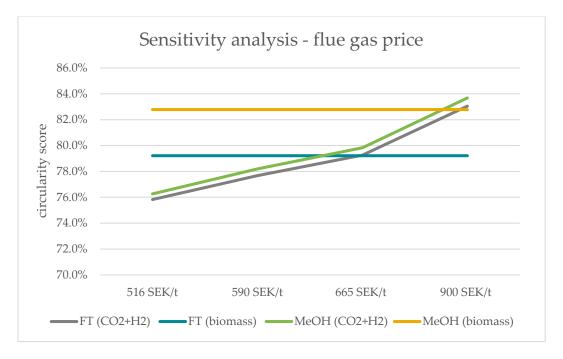


Figure 12. Sensitivity analysis of the circularity score of different value chains to the flue gas price

Figure 12 shows that the increase in the price of flue gas has a positive impact on the circularity score of the FT-crude and methanol produced from CO₂ and H₂. At the price of 657 and 836 SEK/t CO₂, the circularity score of the electrofuels outdo the circularity of the FT-crude and methanol from forest residue respectively.

7 Climate impact and benefit

To assess the environmental impacts and possible environmental gains of the supply chains a life cycle assessment (LCA) with a focus on climate change is performed.

The five value chains included in the LCA are:

Value chain 1: FT crude from hydrogen and carbon dioxide

Value chain 2: Methanol from hydrogen and carbon dioxide

Value chain 3: FT crude from gasification of forest residues

Value chain 4: Methanol from gasification of forest residues and,

Value chain 5: Pyrolysis oil from plastic waste pyrolysis

Goal and scope

The main goal of the LCA is to compare the carbon footprints of the five value chains listed above with their fossil equivalent. The results are also analyzed with respect to hot spots in the life cycle, i.e., which activities contribute the most to the overall carbon footprint.

The functional unit is 1 kg of final product. Value chain 2 and 4 are compared to a conventional methanol produced from natural gas, and value chains 1, 3 and 5 are compared to the intermediate product naphtha. Possible differences in quality between the new value chains and conventional products based on fossil fuels are not considered in this study. The main reason for this exclusion is that data for the value chains are based on theory and literature rather than actual trials and production sites.

The products from value chains 1, 3 and 5 will probably have different heating values compared to each other and the closest fossil equivalent, which has not been considered here either. It is assumed that the closest comparable fossil product to FT crude and pyrolysis oil is naphtha. Depending on the quality of the pyrolysis oil, naphtha may not be the closest fossil equivalent in terms of quality but since no specific production plant is considered here it is used as a proxy. If the quality is low or varying, then a crude oil may be a better proxy than naphtha.

In Figure 13 below, the system boundaries of the value chains are presented.

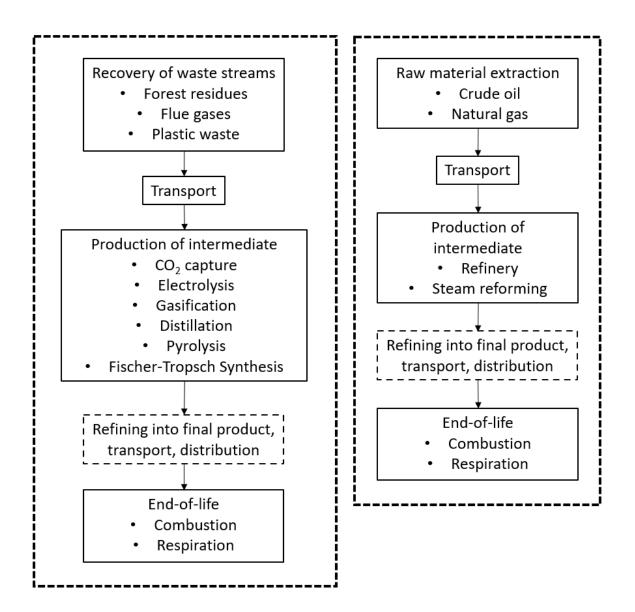


Figure 13. System boundaries of the value chains (left) and their respective fossil equivalent (right).

Waste streams, such as flue gases, forest residues and plastic waste, entering the system boundaries have no upstream burden from previous life cycles. The carbon footprints of fossil equivalents start from and includes extraction of natural gas and crude oil from the ground. Refining of the products FT crude, pyrolysis oil and methanol into final products are not included within the system boundaries, nor the refining of the comparable fossil equivalents.

Downstream emissions resulting from combustion or respiration for naphtha and methanol are included. Depending on where the end products are intended to be used the downstream emissions may or may not be relevant to be included in the assessment. The FT crude, pyrolysis oil, naphtha and methanol may all end up in products which can be recycled or reused at the end of the life cycle thus making the inclusion of downstream emissions irrelevant. However, depending on how many times the materials will be circulated, the material will at the end be incinerated due to quality losses in the recycling loops. To illustrate the inherent differences between raw materials

of renewable and fossil origin, the potential downstream emissions are included in the results. It could however be discussed whether the potential downstream emissions should be a burden on the initial life cycle of the material, or if the burden should be divided equally between all life cycles. Since the use phase if not included here it is impossible to speculate as to how many times the materials can be recycled. If the intermediate products included in this assessment ends up as fuels then the downstream emissions needs to be considered within the scope of this life cycle assessment.

The scope of this study includes one environmental impact category, climate change. Biogenic carbon entering and exiting the system boundaries is excluded since the uptake and emission of biogenic carbon dioxide is net zero over a certain period. It is only the fossil carbon which contributes with a net impact to climate change. The results are expressed as kg carbon dioxide equivalents per functional unit.

Inventory analysis

The inventory analysis is primarily based on the mass and energy balances presented in chapter 7 above. However, the LCA calculations are supplemented with a few process steps and assumptions to complete the life cycle of the value chains such as transports. The main assumptions and limitations of the LCA are presented below:

- The transport distances for forest residues and plastic waste to a recycling facility have been set to 100 km.
- Electricity and heat production in the new value chains are assumed to be produced from renewable sources: electricity from wind power and heat from incineration of biomass.
- The environmental impact of plastic waste collection and sorting, as well as forest residues collection have been approximated with generic LCA data from Sphera (Sphera, 2022) and Ecoinvent (Ecoinvent , 2022) since no specific data is available in this study.
- The environmental impact of further refining and distribution of the products from the value chains have been excluded due to lack of data.
- Downstream emissions from the use of methanol are calculated based on that the total carbon content of methanol is emitted as carbon dioxide.
- Exactly how the FT crude and pyrolysis oil will be utilized is unclear at this stage. It is assumed in this study that the products will replace naphtha, an intermediate product. The downstream emission from naphtha and pyrolysis oil is assumed to be around 3 kg carbon dioxide equivalents per kg, corresponding to incineration of polyethylene.

The LCA modelling has been performed in LCA software and database GaBi (Sphera, 2022).

Results and interpretation

The results are divided into two sets of comparisons: the first where FT crude, pyrolysis oil and naphtha is compared to each other and a second set where methanol production from forest residues, captured carbon dioxide and natural gas is compared to each other.

In the first comparison, presented in Figure 14 below, value chain 1, value chain 3 and value chain 5 is compared to naphtha. Since the pyrolysis oil in value chain 5 is produced from a fossil raw material (plastic waste), downstream emissions are included for this value chain. FT crude in value

chain 1 and 3 is produced from renewable materials (biogenic carbon dioxide and forest residues) the downstream emissions are equal to the carbon uptake in the products, resulting in net zero emissions of carbon dioxide. Downstream emissions from fossil raw materials are marked with a striped field in the figure since it is unclear at this stage how many times the materials will circulate before they are spent and incinerated due to reduced quality. They are included here to demonstrate the potential climate impact of using fossil raw materials rather than renewable materials.

From the figure below, it is easy to see that it is the downstream emissions from combustion of fossil products which have the biggest impact on climate change. If these can be avoided by changing to a renewable raw material or avoided by circulating the material in a closed loop rather than incinerate it, the carbon footprint of the value chain would be decreased by a lot.

When disregarding the downstream emissions and only look at the emissions related to production of the FT crude, pyrolysis oil and naphtha, one can see that value chain 1 and 5 have the highest carbon footprints. In value chain 5, it is the sorting, washing and the reject incineration from the sorting which results in the climate impact from raw material production. In value chain 1, it is direct emissions of methane which gives a relatively high footprint for direct emissions. Value chain 3 has the lowest carbon footprint in this comparison. This is because of an energy integration with a pulp and paper industry.

Production of fossil naphtha has a relatively low carbon footprint due to an effective production which also results in many co-products who share the environmental burden from the refinery.

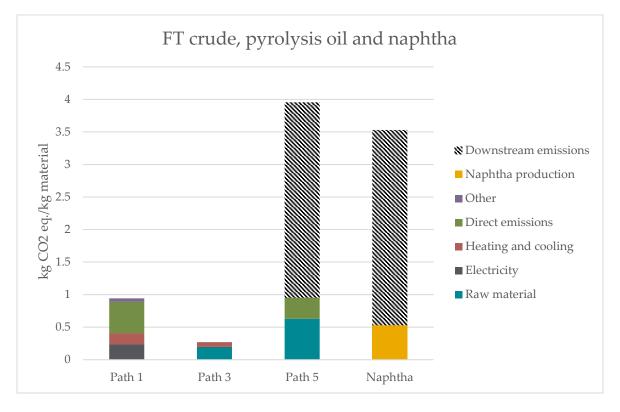


Figure 14. LCA results of the comparison between FT crude from captured carbon dioxide (value chain 1) and forest residues (value chain 3), pyrolysis oil from plastic waste (value chain 5), as well as fossil-based naphtha.

It is however important to remember that the results in this comparison are based on certain assumptions and limitations which can be read in chapter 9.2. For example, it assumed that the FT crude and pyrolysis oil are comparable both to each other and to naphtha. This might not be the case in reality since the quality might differ, especially with regards to the pyrolysis oil. The FT crude is a cleaner intermediate since the raw material is carbon dioxide. Depending on the feedstock for pyrolysis the quality may vary and crude oil might be a better proxy for the fossil equivalent. If the FT crude and pyrolysis oil instead are further refined and used as fuels it might be more relevant to compare to diesel or jet fuel, depending on the material properties. Energy content is not regarded here, and this might be a relevant parameter to compare in the future, especially with regards to pyrolysis oil depending on the feedstock.

In the second comparison, presented in Figure 15 below, value chain 2 and value chain 4 are compared to methanol. Since the methanol in the last column is produced from a fossil raw material (natural gas), downstream emissions are included. Methanol in value chain 2 and 4 is produced from renewable materials (biogenic carbon dioxide and forest residues) the downstream emissions are equal to the carbon uptake in the products, resulting in net zero emissions of carbon dioxide.

As in the previous comparison, it is the downstream emissions from incineration or respiration which contributes the most to climate change. Unlike the previous comparison, and when looking at only the production stage, methanol produced from steam reforming of natural gas has a higher impact than the methanol production from renewable sources. Downstream emissions from fossil raw materials are marked with a striped field in the figure since it is unclear at this stage how many times the materials will circulate before they are spent and incinerated due to reduced quality. They are included here to demonstrate the potential climate impact of using fossil raw materials rather than renewable materials.

Producing methanol (value chain 4) and FT crude (value chain 3) from forest residues have roughly the same carbon footprint per kg of product. Although, more forest residues are needed to produce one kg of methanol compared to producing FT crude.

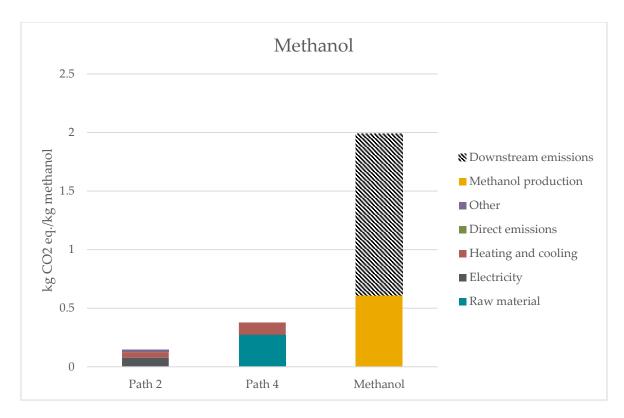


Figure 15. LCA results of the comparison between methanol from captured carbon dioxide (value chain 2) and forest residues (value chain 4), as well as a fossil-based methanol produced from natural gas.

8 Social Sustainability

Sustainability can be defined into three dimensions: environmental, economic, and social sustainability. Social sustainability covers many aspects regarding people's rights and possibilities in a society, both on an individual and on a societal level.

Social sustainability can be assessed both in a quantitative way, which often involves the use of social LCA databases, but also in a qualitative way where the impacts are not measured or calculated.

The social sustainability assessment is based on the results from a workshop held in May 2022 in Åsensbruk, Sweden, with representatives from research institutes IVL Swedish Environmental Research Institute and RISE, Svensk Plaståtervinning, Preem, Scandinavian Envirosystems, Kraton, Walmet and Johanneberg Science Park.

A selection of aspects regarding social sustainability was made by the project team at IVL Swedish Environmental Research Institute together with project members, and the chosen aspects are:

• Job opportunities

- Competence provision
- Gender equality and
- Working environment.

The workshop participants were divided into two groups and discussed different social sustainability aspects in relation to the transition into a renewable and fossil-free chemical industry in Sweden. The results from the workshop are presented in the chapters below.

Job opportunities and competence provision in the plastic recycling business

The first group of the workshop discussed the matters of job opportunities and competence provision in the context of the plastic recycling business and replacing crude oil with pyrolysis oil in a future chemical industry.

New job opportunities for the plastics recycling industry were identified during the workshop, such as sorting and collection of plastic waste, transports of plastic waste but also jobs with regards to research, development, innovations, and industrialization. Since chemical recycling of plastics is a fully new industry, exports of technology, know-how and materials could also increase the number of jobs related to the industry.

According to the workshop participants, the number of jobs will probably be the same as before, possibly a few more. The job opportunities will however be local or regional, rather than national or international. During a transition period, other types of jobs will likely be needed. Jobs in the traditional petroleum industry will instead be replaced by this new industry of plastics recycling. Sustainability and renewable raw materials will likely make the employer more attractive in comparison to the oil and gas industry. This will not affect the number of job opportunities, but may increase the number of applicants for a job.

The types of jobs likely to be requested in a future chemical industry is, according to the workshop participants, lorry drivers, maintenance of mechanical and chemical processes and equipment, process operators, business development and sustainable business models, LCA competence and competence around complex chemical processes, materials, and wastes. It is primarily competence levels which does not specifically demand an academic education to perform which will be needed.

New raw materials will however result in other demands for education. For example, courses with a focus on plastic recycling technologies and refinery of pyrolysis oils will probably be required. This will require economic investments for the actors involved in the new value chain.

Gender equality and working environment in the forestry business

The second group of the workshop discussed the matters of gender equality and working environment in the context of forestry and replacing crude oil with forest residues in a future fossil-free chemical industry.

Compared to oil producing countries, the Nordic countries have a distinct gender equality focus and thus a change in raw materials in the chemical industry would result in a value chain with a better overall gender equality work. However, today the forestry industry in the Nordics is a traditionally male-dominated business and it may prove difficult to renew the gender perspective and to recruit women to jobs which does not demand an academic background. It may turn out to be easier to recruit women to job positions which have a clear focus on sustainability, in comparison to more traditional jobs in the conventional oil and gas industry.

According to the workshop participants, the change to a fossil-free chemical industry may introduce a new opportunity to rethink, redo and break old traditions within the oil and gas industry. This could provide a good opportunity to create a new focus on gender equality. When looking to the future it is however important to consider how gender equality is measured or assessed within an industry or a project and who has the responsibility of following up on a bad gender equality score.

With regards to the working environment, the workshop participants anticipates that the forestry industry in the Nordics generally have a better working environment than the oil and gas industry in oil and gas exporting countries. The participants are divided to whether the forestry industry have more or fewer accidents on site, although it might be more transparent and easier to measure and follow up on in the Nordic countries than in, e.g., the Middle Eastern countries. It may however prove to be difficult to follow the entire code of conduct of suppliers, even though the raw materials are produced locally.

The group identified potential risks when processing a new material, especially when changing from liquids and gases to a solid material. This change requires new tanks, handling procedures, labs, analytical measures etc.

New materials also give rise to new, unknown working environment hazards. For example, oils from different raw materials have different characters and may impose a potential risk when handling it at the site. Oils may have different smells, viscosity, heating values, flash point,



properties when stored etc. New raw materials may also cause unknown effects from longtime exposure.

9 Summary and Discussion

Challenges and mitigation activities

Previous studies have identified challenges for transition to a circular and climate-neutral petrochemical industry. The challenges can be divided into the categories *market barriers, technical challenges, regulatory barriers* and *coordination*. In this study, the focus has mainly been to further investigate the coordination challenges in terms of collaboration and organisational challenges when stakeholders from different sectors need to cooperate in new value chains.

Through the participation of stakeholders from different parts of the value chains, valuable insights have been developed. The challenges are found to be on both practical level, such as lengths of contracts and quality specification, and more philosophical level, such as conflicting sustainability goals. As an outcome from discussions between the stakeholders, mitigating activities have been identified for most of the challenges. To a large extent, the mitigation activities involve establishing platforms for collaboration, both for technological development and discussions about standards, logistics, permits and other common issues.

However, several topics remain to be explored in future studies. For example, the market requirements for guarantee of origin for bio-based or circular raw-material could be studied in relation to the technological options for different value chains.

Financial barriers do not seem to be a big concern. The participating parties believe that good ideas in the area of the new value chains will be able to finance needed capital investments. This result is in line with (Maltais, Karltorp, & Tekie, 2022) who confirms this as they conclude that neither the scale of capital investments in deep green industrial transition in Sweden nor access to financing to make these investments are perceived to be significant obstacles by industry or financial actors. However, a financial challenge identified by (Johansson, et al., 2021) and (Fossilfritt Sverige, 2022) is that although there are many possibilities in terms of public support for research, development and demonstration of innovative technologies, both at national and international level, it can be challenging for an individual actor or a collaboration project to get an overview of these possibilities as well as what entities/authorizes to contact. In (Johansson, et al., 2021) actors in the chemical and refinery industry express their view on this and point particularly to difficulties of applying for funding at the international level.

The results from this study also highlights is the importance of considering the global competition within firms. This is in line with the findings of (Bauer & Fuenfschilling, 2019) who investigate the interrelations between global regimes and local sustainability initiatives. They find that internal competition for resources might limit the possibilities to fund and pursue local innovative projects as priorities are set by distant headquarters

A division in viewpoints can be seen between small and large stakeholders. In general, the small stakeholders are dependent on the large for off-take for their products. Hence, they are concerned about contractual lengths and product specifications. In order to upscale production, the firms need to know that they have an off-take of their product for a long time, but e.g. in the refinery industry there is a tradition of short contract periods. Some of the smaller firms involved in the project has also raised concerns about protection of their intellectual property when collaborating closely about technical development with large firms.

Mass and energy balances

Table 10 shows the overall input needed to produce 1 kg of product of interest, i.e FT-liquid, methanol, and pyrolysis oil. Table 11 shows the overall energy balances. Value chains 1, 3 and 4 where integrated with another type of industry to exchange material and energy streams. A description of the different value chains is presented in Chapter 7. In this chapter, value chains starting with the same raw materials are compared to each other. Therefore, value chain 1 and 2, and value chain 3 and 4 are compared. Value chain 5 will be discussed with value chain 1 and 3 because of the end product similarity in heating value.

As seen in Table 10, value chain 1 and 2 start with the same raw materials CO₂ and H2 but produce two different products, ie. FT-crude and Methanol. FT-crude is used as fuel (Speight, 2020) while methanol is used for both fuel and as a building block for producing more complex chemicals (Dalena et al., 2018). The energy density of methanol (LHV: 20.1 MJ/kg (Szima & Cormos, 2018)) is almost half of that of FT-liquid (average LHV: 43 MJ/kg (Fagerström et al., 2021)) and that is why methanol has traditionally been used more in the production of other chemicals rather than as a fuel. Nevertheless, the implementation of legislation such as RED II from the European Union, promotes and creates a market for renewable fuels such as methanol (European Parliament & Council of the EU, 2018) (Irena and Methanol Institute, 2021)

When it comes to material intensity, methanol production is less intensive than FT-crude production. This can be explained by both chemistry and efficiency of the processes. Methanol is a molecule that contains oxygen atoms which come directly from the CO₂. FT-crude contains mainly hydrocarbons of different chain length and in a less portion oxygenates (Neste & VTT, 2019) since the main FT reaction is between CO and H₂ and the oxygen in CO ends up in the by-product water molecule. The efficiency of the process is also higher for the methanol (97% of CO₂) compared to that of FT -crude (60-90% of CO). Since less CO₂ is needed for the methanol synthesis, less MEA (30%wt) is needed. When it comes to H2, in the production of FT-crude, H2 is needed in larger quantities because it is present in the long chain of hydrocarbons that constitute the crude. Furthermore H₂ is consumed in the rWGS reaction to form CO. The water consumed is for the MEA and the electrolysis and since there is more H₂ and MEA for the FT-crude production, more water is also needed in the FT-crude production than for the methanol production.

The value chains 3 and 4 start with the same raw materials forest residues and O_2 but produce two different products, i.e FT-crude and Methanol. In this case, the use of forest residues is higher for the methanol production. This can be explained by the fact that methanol is a pure final product while FT-crude needs further refinement where H₂ is required, and thus material is added downstream.

Finally, for value chain 5, since both raw material and end product are different from the other value chains, the only similarity that can be used to compare it to the other value chains is the heating value. The pyrolysis oil has a low heating value of 41-44 MJ/kg. This value is similar to that of FT-liquid (43 MJ/kg). For the same amount of product, the material usage is less for value chain 5 than value chain 1 and 3. However, since the raw materials and the source are different, the comparison might need a more detailed analysis such as the one done in the LCA.

Table 10: Relevant inputs and outputs from all value chains normalized to 1 kg of product

	Raw materials	Product			
Value chain 1	Water	MEA	CO ₂	H ₂	FT-crude

	6.88 kg	0.02 kg	4.13 kg	0.58 kg	1 kg
Value chain 2	Water	MEA	CO ₂	H ₂	Methanol
	2.46 kg	0.01kg	1.55 kg	0.19 kg	1 kg
Value chain 3	Forest residu	ies (50% MC)	O 2	H ₂	FT-crude
value chain 3	11.1 kg		1.9 kg	0	1 kg
Value chain 4	Forest residues (50% MC)		O 2	H ₂	Methanol
Value Chain 4	16.2 kg		2.8 kg	0	1 kg
Value chain 5		Pyrolysis oil			
value chain 5		1 kg			

Note: The CO2 in value chains 1 and 2 correspond to the CO2 captured in the CO2 capture unit. The water refers to the water needed for electrolysis and for the MEA solution at 30% wt. The H2 is the one produced after electrolysis in value chain 1 and 2.

For the energy demand, value chain 1 and 2, and value chain 3 and 4 are compared to each other. Value chain 5 is discussed alone since the scale as well as the raw material and end product is different and information is scarce.

As can be seen in Table 11, value chain 1 has a higher overall energy demand. For value chain 1, the biggest demand of electricity is required for the production of H₂ by electrolyzer (86%). As seen in Table 10, the H₂ consumption for value chain 1 is larger than in value chain 2. When comparing the heat demands, it should be noted that value chain 1 was integrated with a CHP plant while value chain 2 was not integrated but used an organic rankine cycle and a steam recovery cycle to cover the majority of its demand. Nevertheless, the heat required for value chain 1 is higher than value chain 2. This can be explained by the demand of the rWGS reactor which is needed in value chain 1 but not in 2. When it comes to cooling demand, value chain 1 also has a higher demand, corresponding to electrolyzer and the rWGS reactor. However, part of the heat that requires cooling is delivered as district heating. It is important to consider that when it comes to delivering heating to the district heating as a form to reduce the cooling demand of the process, this can only be done in countries that uses district heating, such as Sweden.

As seen in Table 11, the overall energy demand of value chain 3 is higher than value chain 4. It should be noted that both processes were integrated to a chemical cluster, and both have a heat recovery steam cycle. In value chain 3, the integration with the cluster was done by the transfer of heat from gasification to the FT-crude refinement process (which was done by the cluster). Nevertheless, heat is required for drying of the biomass. From value chain 2, heat from the gasification process is also deliver to the cluster and drying was done by the cluster. When it comes to cooling, the biggest demand in value chain 3 comes from the methanol synthesis while in value chain 4 comes from the FT synthesis reactor.

For value chain 5, the data obtain was from lab scale. Nevertheless, it is known that the combustion of the pyrolysis gas, which has a heating value of 45 MJ/kg, can be used to run the process. For the cooling demand, a lot is needed for the condensation of the gases that come from the pyrolysis reactor.

	Energy needed per kg of product					
	Electricity	Heating	Cooling			
Value chain 1	34 kWh	7.8 kWh	19.5 kWh			

Table 11: Overall energy demand of all value chains per kg of product

Value chain 2	11.16 kWh	2 kWh	7.25 kWh
Value chain 3	1.5 kWh	3.5 kWh	3.4 kWh
Value chain 4	0.5 kWh	-	5.0 kWh
Value chain 5	Possibly self-sufficient gases that produce ste	,	Probably a high demand to condensate the pyrolysis gases

Some if the technology used in the mentioned value chains has already been in use for the refinery and chemical industry. The major obstacles for the large-scale production for the different routes is the higher product price compared to fossil fuel-based products. This are due to high electricity prices, technology readiness of some of the process steps and high heating and cooling demands. One way to tackle these challenges is by using existing infrastructure and integrating the process to industrial parks as well as by continue the development of the different technologies.

Circularity benefit

The circularity of the five value chains was evaluated based on the use of renewable inputs and secondary resources in the product, expressed by renewability and recycled content indicators. To obtain these two indicators for the output of a process of stage, weighted aggregation method based on economic value was used. The results shows that the more share of renewable material and secondary resources used in the product, the higher the circularity. Inputs with a high recycled contents are typically those that have been waste once. Hence, a high circularity also indicates that low quality input materials are efficiently transformed into a product with higher value.

As two indicators are used, an aggregating method is needed. In this study, economic value was chosen as the common property between the mass and energy inputs. The sensitivity analyses shows that the circularity of each value chain also depend on the prices of each input. Increase in prices of electricity that are not 100% renewable gives negative effect to the circularity of the products that are more energy intensive e.g. products from CO₂ and H₂. A higher price on waste on the other hand contributes to a higher circularity. This makes the circularity assessment method being somewhat vulnerable which can cause the results to have some uncertainty.

The level of detail of the input materials and energy plays an important role in the assessment. For the case of pyrolysis oil, the only input considered is the plastic waste as the energy demand was assumed to be supplied internally by its co-products. As such the circularity score for the pyrolysis oil only reflects the upgrading of the plastic waste. Since the plastic waste was estimated to have a low share of biomass, the circularity score of the pyrolysis oil was also low. For the gasification process of biomass, inputs such as fluidized bed material is not included. As this bed material is likely to have a low renewability and low recycled content, it is likely that adding this input in the calculation will lower the circularity score of the value chains that are based on this process.

When changing the renewability of the electricity to 100% in all value chains as part of the sensitivity analyses, the results shows that the circularity score increases significantly, especially for the value chains that are energy intensive. However, it still does not change the overall results of the study. Namely, that the value chains with CO₂ and H₂ has a lower circularity score than those based on forest residue. If a 100% renewable electricity can be used together with a low price of electricity, the resulted circularity benefit would be high.

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Furthermore, an average was used when weighting the renewability and recycled content indicator of the final product into one circularity score. This means that both indicators are valued equally for the circularity benefits. However, this weighting can change depending on the importance of each indicator. If the recycled content is to be prioritized, then the final circularity score will be different. However, as the value chains based on forest residue have higher renewability and recycled content, changing the weighting factor will only affect the magnitude of the circularity score but not the order of which value chains are preferred.

It can be said that there is room for improvements in the assessment of the circularity benefits in this study. Firstly, the level of detail in the input-output data should be expanded to include other inputs other than the raw materials such as chemicals, auxiliary materials, catalyst and bed material. Increasing the level of detail in the calculation will give a better picture of the circularity of the value chain. Include transportation in the value chain will also contribute to a better evaluation. However, to be able to do this, a specific value chain with specific data for each process will be needed. Secondly, the adopted method was initially developed to evaluate the circularity of transportation fuel. This means that it does capture the recyclability of the products. In addition, since the method is based on material and energy input, energy integration within the system is not captured either. Developing a way to include these two aspects would greatly complement this evaluation method.

Note that the definition of circularity used for the quantitative analysis in this report, only reflects the origin of raw materials, if they are from renewable sources or from recycled material. What it does not reflect is the downstream circularity, such as recyclability.

The value chains that are analysed in this report, are not the complete chains. They start from the raw materials, go through processes to an intermediate product, a crude oil or methanol. Hence, the continuation of the value chain such as the further processing to fuels, plastics etc., and even further to consumer products, is not included. This is interesting to complement with in further research.

Climate impact and benefit

The climate impact assessment showed a potential climate benefit when changing from fossil raw materials to renewable. When analysing the results, it is however important to remember that the LCA is performed in an early stage of development and data is not based on actual measured data from an existing industry or production plant. As an example, only intermediate products are included in the assessment (Fischer-Tropsch crude, pyrolysis oil and methanol) and no refinery of the intermediates is included at this stage due to lack of information.

In the future, it would be of interest to include the refinement of the products since this would enable a comparison of different product qualities and to perform a comparison with a more relevant fossil equivalent. By including the refinement and basing the inventory data on an existing plant it is possible to achieve a clearer picture of the climate impact but also to answer the question of what or which fossil equivalents are being replaced by this renewable fuel or raw material in the chemical industry.

Since the LCA is performed in an early stage, it is difficult to assess whether all inventory data have been included in the analysis since it is not possible to check the values with an existing

production plant. The results do, however, indicate that by changing to renewable raw materials the climate impact will decrease. The effect is not visible at this stage, and in combination with the chosen system boundaries, for changing fossil raw materials to pyrolysis oil from plastic waste.

Social sustainability

A first attempt in assessing the social sustainability of a future, fossil-free chemical industry was performed in this study. Business experts and researchers participated in a workshop to brainstorm and discuss a selection of social aspects in a change from fossil to renewable raw materials in the chemical industry of the future. A selection of relevant aspects was made to facilitate a good discussion amongst the workshop participants, and the selection were made in cooperation with the BeKind project group. This selection forms a limitation in this study since there might be other important aspects regarding social sustainability which might not be addressed in this study. Examples of aspects which are not addressed here are human rights, diversity, and inclusion.

At this stage, the social sustainability assessment is qualitative, not quantitative, meaning that it is not possible to compare the effect of gender equality and job opportunities in this study in any way. To quantify the social aspects in an S-LCA (Social Life Cycle Assessment) could provide an answer to what or which aspects could be the most important to focus on improving when changing from a fossil to a renewable chemistry industry in the future. As in the case of the LCA, having data based on a real case study or production plant could improve the input data quality to the S-LCA as well as provide a clearer answer as to which social aspects are most important to focus on in this transition.

10 Conclusions

Challenges and mitigating activities

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The transition to a circular and climate-neutral petrochemical industry involves challenges on several levels since firms from different sectors that have not collaborated before will need to collaborate. In general, a great amount of work needs to be performed in terms of forming partnership and platforms where the challenges can be handled.

Development of new technology is often in the outskirt of the firms' core business. In order to share risks of investment and keep up the pace in long-term development, the forming of partnerships and founding of joint ventures are parts of the solution.

Practical issues such as over-specification of quality for raw materials and the length of contracts needs to be solved through agreements between the stakeholders. The specifications need to be reviewed by the owner of process equipment. In general, smaller firms are more concerned about their dependency on large actors and need assurance that they have an off-take for their products.

With regards to circularity and handling of waste, there is a demand for more regulation and agreements regarding the logistics.

In addition, a market challenge was highlighted in the discussions between stakeholders. The enduser's requirements on material origin may conflict with the technical opportunities within the industries, specifically the mass-balance method may not be accepted in all product or end-user segments. This is an interesting issue which needs to look further into. Public procurement and certification of origin in relation to the possible technological options could be explored in future studies.

Mass and energy balances

From the analysis of the material balances, it could be concluded that Methanol is less material intensive than FT-crude when the starting feedstock is CO₂ and H₂. This is explained by the chemistry of the end-products and the efficiency of the processes. Nevertheless, the energy content of the FT-crude is higher than methanol which is an advantage for the usage as fuel. On the other hand, Methanol appears to be more material intensive than FT-crude starting from forest residues as feedstock. Nevertheless, if refinement would be added to the assessment, then FT-crude would again need more material since H₂ would be supplied.

From the analysis of the energy balance, it was seen that, starting from CO₂ and H₂ FT-crude production required more energy than methanol production. FT-crude was integrated with a CHP plant that provided heat while methanol uses an organic rankine cycle and a steam recovery cycle.

The largest consumer of electricity was the electrolyzer and the largest consumer of heat was the rWGS reactor which is absent in the methanol synthesis. The largest consumers of cooling are also electrolyzer and rWGS reactor. Some if this cooling is achieved by delivering the heat to the district heating. When it comes to the production of methanol and FT-crude from forest residues, both value chains were integrated to a chemical cluster. The FT-crude value chain delivered part of their waste heat to the cluster while the methanol value chain used the heat from the cluster to dry the biomass. Both value chains also had a heating recovery cycle which in the case of methanol

production covered the heating demand. The cycle gases were also used to produce electricity. The integration with a cluster reduced considerably the energy demand.

Circularity benefits

While there are many definitions of circular economy, the evaluation method used in this study defines the circularity benefits as something that derive from renewable and recycled materials. Product that has a high circularity score indicates an efficient process where low quality inputs are upgraded into a higher quality output.

The results from the evaluation of the circularity benefits shows that the value chain that has high share of renewable material and recycled content contributes to a high circularity. In this case, the FT-crude and methanol produced from gasification of forest residue has the highest circularity score which are 79% and 83% respectively. Both FT-crude and methanol from CO₂ and H₂ received a circularity score of 78%. The pyrolysis oil which contains a low fraction of bio-based plastic has the lowest score of 51%.

In addition to the renewability and recycled content indicators, the circularity score is also depending on the price of the inputs. As prices can vary depending on supply and demand, this assessment method is deemed to have some uncertainty. The circularity benefit evaluation can be improved by increasing the level of detail of the material and energy inputs and outputs in order to capture the whole picture of the value chain as well as to lower the uncertainty of the result.

Climate impact and benefits:

The results from the climate impact assessment indicate that it is beneficial to change from fossil raw materials (petroleum and natural gas) to renewable (forest residues and captured carbon dioxide) in the context of chemical industries. The results do not indicate a climate benefit in the case of pyrolysis oil from plastic waste in comparison to a fossil equivalent produced from primary resources. By using renewable resources, downstream emissions of fossil carbon dioxide from incineration could be avoided. By integrating production processes in industrial symbioses less external energy is needed and thus resulting in a lower carbon footprint.

Social sustainability

The workshop participants concluded that in the case of job opportunities and competence provision in the plastics recycling business that the number of jobs will probably be the same or close to the same as before. New job opportunities will for example appear as process operators, maintenance operators and lorry drivers, but also jobs relating to research, development and industrialization.

Regarding the matter of gender equality and working environment, the workshop participants concluded that a transition into renewable raw materials could provide a window to rethink and redo old traditions within the forestry business in the Nordic countries.

The workshop participants also concluded that there are potential working environment risks related to processing new materials when changing from liquids and gases to solid materials. This requires new equipment and analyses. New materials also increase the risks for unknown working hazards within the forestry business and chemical industry.

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