Future alternative transportation fuels

A synthesis report from literature reviews on fuel properties, combustion engine performance and environmental effects

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Sammanfattning

Enligt EU ska utsläppen av växthusgaser minskas med 60% till år 2050 (jämfört med 1990 års nivå) och i transportsektorn ska alla medlemsländer ha 10% förnybara drivmedel år 2020. I Sverige har regeringen uttalat en vision om att åstadkomma ett energisystem utan nettoutsläpp av växthusgaser till år 2050 och en fossiloberoende fordonsflotta år 2030, där tolkningen av den sistnämnda är fastslagen till en reduktion av växthusgaser från vägrafiken med 80% jämfört med 2010. Syftet med den här studien är att genom litteraturanalyser nå en ökad förståelse för komplexiteten kring omställningen från dagens konventionella drivmedel till användning av framtida nya drivmedel liksom hur man identifierar bränslekandidater som har utmärkta förbränningsegenskaper och samtidigt är mer miljövänliga än dagens bränslen.

En viktig del i analysen är att förstå hur stor mängd biodrivmedel som kan produceras på ett hållbart sätt. Från litteraturen drar vi slutsatsen att upp till 100 EJ bioråvara kan produceras på ett hållbart sätt i världen. Om vi antar att hela denna bioråvara omvandlas till biodrivmedel med en omvandlingseffektivitet på ca 50% kan vi fastslå att maximalt 50 EJ hållbara biodrivmedel kan bli tillgängligt för världens transportsektor. Som jämförelse så används ca 100 EJ transportbränslen i världen idag. För Sverige ser vi att det kan vara möjligt att producera 20–35 TWh biodrivmedel per år från inhemsk bioråvara, vilket kan jämföras med dagens användning av bränslen för vägtransporter på ca 80 TWh/år och ca 100 TWh/år för hela den svenska transportsektorn.

Det finns ett flertal utmaningar kopplade till en global uppskalning av produktion av biodrivmedel. Globala utmaningar behöver däremot inte nödvändigtvis gälla för den svenska produktionen. Fördelar för svensk biodrivmedelsproduktion är till exempel att det finns en stor mängd bioråvara i form av restprodukter från ett omfattande skogsbruk, en väl utbyggd infrastruktur för hantering av stora mängder bioråvara som byggts upp kring svensk massa- och pappersindustri, en väl utbyggd tankstationsinfrastruktur för etanolbränslet E85 liksom att Sverige är ett glest befolkat land vilket indikerar att det inte är någon omedelbar brist på mark för framtaganing av bioråvara.

I ett kort tidsperspektiv visar litteraturanalysen att SI-motorer arbetar ännu bättre på vissa alkoholbaserade drivmedel än på bensin. Negativa aspekter är kallstartsegenskaper, korrosionsproblem och det lägre värmevärdet som gör att fordonet behöver större bränsletankar. En blandning av molekyler, med olika tändegenskaper, är generellt fördelaktigt för att underlätta kallstarter. En blandning av bensin, etanol och metanol är en sådan blandning som skulle förbättra kallstartsegenskaperna och som dessutom skulle kunna distribueras i existerande E85-infrastruktur och användas i konventionella SI-motorer. När det gäller dieselmotorer så ser vi att HVO och alkoholer är de drivmedel som har hög relevans att studera för användning i en nära framtid. Överlag ser vi vikten av att öka utvecklandet och användningen av drop-in-bränslen i både diesel och bensin under en övergångsperiod där man stegvis fasar ut mängden fossila bränslen.

I ett längre tidsperspektiv finns det möjlighet att anpassa bränslen och motorkoncept till varandra. Tester som gjorts med motorkoncept under utveckling såsom HCCI, RCCI och PPC visar på både högre verkningsgrad och lägre utsläppsnivåer än konventionella bensin- och dieselmotorer. Dessa framtida motorkoncept visar också fördelaktiga utsläppsvärden när de körs på alternativa drivmedel. En möjlighet är att identifiera ett bränsle med förbränningsegenskaper mittemellan bensin och diesel. som kan optimeras för användning i anpassad PPC-motor. Ett lovande framtida bränsle för en DICI

motor skulle kunna vara POMDME. Även alkoholblandningar för användning i DICI-motorer verkar vara lovande.

Goda bränslekandidater, från ett förbränningsmotorperspektiv, kan identifieras genom att till exempel titta på molekylens uppbyggnad. Molekyler som innehåller syre har en tendens att minska sotbildningen i förbränningen. För att undvika alltför stora bränsletankar är det också en fördel om bränslet har ett värmevärde högre än 30 MJ/kg. En kokpunkt mellan 50–100 ºC är också eftersträvansvärt efter som en låg kokpunkt ger en snabb spray brake-up och spridning av bränslet i förbränningsögonblicket. Vidare är det önskvärt att bränslet har en låg koncentration av aromater eftersom dessa har en tendens att öka partikelutsläppen vid förbränning.

Identifierade lovande bränslekandidater är till exempel alkoholer med kolkedjor mellan C_1–C_{10} , etrar speciellt di-n-butyleter (DNBE) och POMDME ($CH_3O(CH_2O)nCH_3$), farnesenes i antingen raka eller förgrenade kolvätekedjor, levulinate och furoate kan bli viktiga inblandningskomonenter, 2-butanon som verkar ha liknande egenskaper som etanol men fungera bättre vid kallstarter, och 1-oktanol.

Från ett produktionskostnadsperspektiv är det fördelaktigt om bränslet antingen (1) är en liten molekyl som kan syntetiseras från mycket små byggstenar som tex CO och H2 i syngas, (2) är en molekyl som liknar de molekyler som finns i biomassa, eller (3) är en molekyl som redan massproduceras i kemikalieindustrin. Från litteraturanalyserna med fokus på ett övergripande systemperspektiv vi ser att inget enstaka bränslealternativ har kunnat identifieras som en vinnande kandidat. Det är istället troligt att en mängd olika bränslen kommer ut på marknaden. Generellt sett ses bränslen som kan blandas med konventionella drivmedel som fördelaktiga, liksom om bränslen kan produceras utifrån avfall, restflöden och inhemsk bioråvara. För Sverige ses bränslen baserade på restflöden från skogsbruket som lovande alternativ.

Den övergripande utmaningen är att kunna producera alternativa drivmedel på ett ekonomiskt hållbart sätt utan behöva subventioner i framtiden. Fördjupade kunskaper behövs kring osäkerheter kopplade till vilka bränslen som har framtiden för sig och vilka som dras med stora utmaningar. I detta arbete behöver både bränsle- och fordonstillverkare involveras. Detta indikerar att det finns ett behov av tvärvetenskaplig forskning som genom ett iterativt arbete kan kvantifiera bränsleproduktionspotential, energibalanser utsläpp av växthusgaser i ett well-to-tank perspektiv liksom beräkningar av total kostnad. Detta arbete behöver göras i samverkan och i öppna studier för att få alla aktörer involverade, vilket ökar möjligheten att få acceptans för resultaten.

Executive summary

According to EU, all transport related greenhouse gas emissions must be reduced by 60% by 2050 (compared to 1990) and 10% renewable energy should be used in the transport sector by 2020. The ambitions of the Swedish Government is an energy system without net emissions of greenhouse gases by 2050 as well as a vehicle fleet, for road based transport, that is independent of fossil fuels by 2030. The aim of this study is, through literature review, to reach a better understanding of the complexity around the transition from conventional oil-based fuels to future alternative transportation fuels and how to identify fuel candidates with excellent combustion properties that also are better than conventional fuels from an environmental perspective.

One important factor is to understand the amount of biofuels that can be produced in a sustainable way. In the reviewed literature we find that up to 100 EJ of primary biomass seems possible. Assuming that all of this biomass will be used for the production of biofuels for transport, and accounting for around 50% conversion losses, we conclude that maximum 50 EJ of sustainable biofuels may be available for the global transportation sector. This can be compared to a currant global demand for transportation fuels of 100 EJ. For Sweden, the biomass supply potential limits the biofuel production to 20–35 TWh/year, which is around a third of current fuel demand.

There are multiple challenges connected to a globally large-scale expansion of biofuel production. These may, however, not necessarily apply to an increased biofuel production in Sweden. Advantages for Swedish biofuel production are the availability of forestry residues, a well-established infrastructure for handling large volumes of biomass (from a long tradition of pulp and paper industry), a built out refueling infrastructure for E85 as well as Sweden being a sparsely populated country implying no immediate land scarcity.

In a short term perspective reviewed literature shows that SI engines work even better on alcohols than on gasoline. Negative aspects are cold start performance, corrosion issues and increased volumetric fuel consumption. A mix of molecules with different ignition properties in the fuel is beneficial for cold starting issues. Ternary blends of gasoline, ethanol and methanol are such mix of molecules that would improve cold start issues. Ternary blends can further be used in conventional combustion engines and the existing distribution system of E85. On the DICI engine side HVO as well as alcohol mixtures seem the most relevant ones to investigate further in the short term perspective. For the short term future it seems relevant to increase the amount of drop-in fuels in gasoline and diesel to eventually phase out the fossil fuels in the mixtures.

In a longer term perspective there is an opportunity to adapt both fuels and engines to each other. The emerging combustion concepts HCCI, RCCI and PPC demonstrate both higher efficiency and lower emissions than conventional SI or DICI. These concepts do also provide emission benefits when operated on alternative fuels. One such opportunity would be to find alternative fuels and blends that can be matched with PPC engine adaption, where fuels with combustion properties somewhere in-between gasoline and diesel seems promising. For DICI engines POMDME and its derivatives are candidates that at least theoretically could be good for clean DICI operation. Ternary blends are also relevant for DICI where a baseline specification should be sought and investigated.

Good fuel candidates, from a combustion perspective, can be identified by e.g. checking the atom content in the fuel molecule since it is shown that fuels that have oxygen integrated in the molecule tend to decrease soot formation, and to avoid large fuel tanks it is beneficial with a fuel that have a heating value larger than 30 MJ/kg. A boiling point between 50–100 ºC is beneficial since a low boiling point leads to rapid spray brake-up and mixing in the combustion. Further, low concentration of aromatics is advantageous since they tend to increase emissions of particulate matters.

Identified promising future fuel candidates are e.g., alcohols in the range C_1–C_{10} , ethers, especially di-n-butylether (DNBE) and POMDME ($CH_3O(CH_2O)nCH_3$), farnesenes in either straight or branched olefin hydrocarbon chains, levulinate and furoate could be important as blend components, 2-butanone with similar properties as ethanol but better cold start performance and 1-octanol.

From a production cost perspective it is beneficial if the fuel either (1) is a small molecule that can be synthesized from syngas or similar processes or (2) a molecule that is similar to molecules in biomass or (3) already is a large scale produced chemical. From the systems studies perspective no single fuel is identified as winning alternative. It is likely that a mixture of alternative fuels will enter the fuel market. Fuels that can be blended into conventional fuels are generally seen advantageous, as well as fuels that can be produced from waste streams or locally available bioenergy sources. For Sweden, fuels based on forestry residues are seen as promising options.

The overall challenge is to make alternative fuels economically competitive without subsidies. The insecurity regarding which fuel has a future and which are facing major challenges need to be better understood. The vehicle manufacturers have to be involved in the process as well as the fuel producers. This implies that there is a need for interdisciplinary and iterative system and engine research that can quantify the production potential, well-to-tank carbon emissions as well as total cost calculations. The computations have to be made transparent in order for the industry to be involved and accept the results.

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Abbreviations

BTE – Brake Thermal Efficiency
CFPP – Cold filter plugging point
CI – Compression ignition engines
CO – Carbon monoxide
CO_2 – Carbon dioxide
CH_4 – Methane
CNG – Compressed Natural Gas
DI - Direct injection
DICI - Direct injection compression ignition (the conventional diesel engine)
dLUC – direct Land Use Change
DME – Dimethyl ether
EATS – Emission after-treatment systems
EGR – Exhaust Gas Recirculation
FAME – Fatty acid methyl ester (biodiesel based on vegetable oil, e.g. rapeseed)
FT-fuels – Fischer Tropsch fuels
GIE - Gross indicated efficiency
GTL – Gas to liquid
H_2 – Hydrogen
HC - Hydrocarbons
HCCI - Homogeneous charge compression ignition.
HD – Heavy Duty (usually refers to trucks)
HVO – Hydrotreated vegetable oil (biodiesel that can be based on talloil)
ICE - Internal combustion engine
iLUC – indirect Land Use Change
LD – Light Duty (usually refers to cars)
LNG – Liquefied natural gas
LUC – Land Use Change
NOx - Nitrogen oxide emission
POMDME - Polyoxymethylene Dimethyl Ethers (also known as PODE or DMMn)
PPC - Partially premixed combustion
RCCI - Reactivity controlled compression ignition
RME – Rapeseed methyl ester
RON - Research octane number
SI - Spark Ignited (the traditional gasoline, Otto, engine)
SME – Soy methyl ester
TWC – Three Way Catalyst
WTT – Well-To-Tank

Introduction

This is a synthesis report for an interdisciplinary pre-study on future alternative transportation fuels. The pre-study is a collaboration between combustion researchers at three large technology universities in Sweden (KTH, Chalmers and Lund University), system perspective researchers and representatives from the industry.

Background

Passenger and freight transportation contributes globally to 19% of energy use and 23% of energy related CO_2 emissions (IEA, 2009). Many projections indicate that energy use and CO_2 emissions from transport could rise sharply in the future (IEA, 2010; Schafer *et al*, 2010). In order to reach ambitious climate targets global greenhouse gas emissions need to be substantially reduced in all energy sectors. The amount of CO_2 emitted from the transportation sector depends on the amount of energy used (energy demand) and how much CO_2 that is emitted from each energy unit used. The energy demand depends on the amount of vehicle kilometer driven and the amount of energy used per kilometer. Nine examples of how to reduce emissions from the transportation sector are presented in Figure 1.

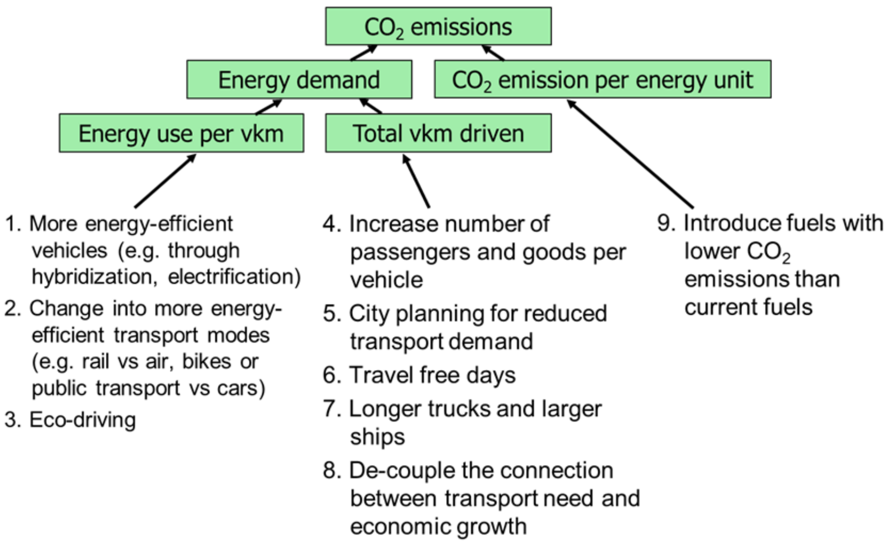

Figure 1. Example of measurements for how to reduce CO_2 emissions from the transportation sector.

According to EU white paper from 2011 all transport related greenhouse gas emissions must be reduced by 60% by 2050, compared to 1990 (European Commission, 2011) and in the directive 2009/28/EC of the European Parliament and of the council it is stipulated that all EU member states should have 10% renewable energy in the transport sector by 2020 (European Parliament and Council, 2009).

In addition to EU policies, Sweden has and has had several national policies stimulating the production and use of renewable fuels for transport, as well as policies for associated vehicles, e.g., energy and carbon tax exemption for renewable fuels, vehicle tax exemption for green cars (replacing a green car premium), benefits value for certain green cars, obligation for fuel retail outlets to offer renewable fuels, investment aid for biogas and other renewable gases, carbon dioxide (CO_2) differentiated annual vehicle tax, super green car premium (mainly for electric vehicles) and a quota system for biofuels for transport is expected to become operative in the near future (Government Offices of Sweden, 2011; Grahn and Hansson, 2015). However, the energy and carbon tax exemption rules have recently become less generous mainly because tax exemption has become costly for the Government (Swedish National Audit Office, 2011) which can be seen as an indication of renewable fuels expanding on the market.

The ambitions of the Swedish Government is a sustainable and resource efficient energy system without net emissions of greenhouse gases to the atmosphere by 2050 as well as a vehicle fleet, for road based transport, that is independent of fossil fuels by 2030 (Government Offices of Sweden, 2009). Following these two ambitions, results from the Swedish governmental investigation, called "Utredningen om FossilFri Fordonstrafik" (FFF-utredningen), show (1) a substantial reduction in the amount of vehicle kilometer driven and the amount of energy used per kilometer, (2) that electricity will expand as an energy carrier in the transportation sector and (3) that large amounts of biofuels will be used in Sweden in 2030–2050 (Johansson, 2013).

Other scenario studies have also pointed out the importance of changing to renewable transportation fuels to be able to reach ambitious CO_2-reduction goals and the global 2 degree target (e.g., Olsson *et al*, 2013; Swedish Transport Administration, 2012; Grahn *et al*, 2009).

Aim of this study and structure of this report

The aim of this study is, through literature review, to reach a better understanding of the complexity around the transition from conventional oil-based fuels to future alternative transportation fuels and how to identify fuel candidates with excellent combustion properties that also are better than conventional fuels from an environmental perspective.

The literature review has been divided into three topics: (1) alternative fuels for internal combustion engines – focusing on fuel properties, (2) combustion of alternative vehicle fuels in internal combustion engines – focusing on results from experimental research, and (3) systems perspectives on alternative future transportation fuels – focusing on challenges and possibilities for biofuels in a wider perspective. Results from the literature reviews are presented in three free-standing reports (Holmborn, 2015; Tunér, 2015; Heyne *et al*, 2015).

This is the fourth report, within our pre-study, and contains a synthesis and some suggestions for future research. After the introduction section in this report we have included a section describing the Swedish transportation sector followed by two sections (feedstock and bioenergy supply potential as well as fuel production) which contain summaries from Heyne *et al* (2015). In the section about fuel production we have also added a description of electrofuels. The section about fuel properties summarizes the major results from Holmborn (2015) and thereafter a short section on health effects of fuels followed by the main results from Tunér (2015) about engine performance. The section following engine performance covers the well-to-wheel analysis and system perspectives based on Heyne *et al* (2015). Thereafter we present lessons learned from the project on tailor-made fuels at RWTH Aachen University in Germany. The report ends with a discussion section that summarizes the reflections made in the three other reports as well as conclusions and identified knowledge gaps and research needs.

Swedish transportation sector

Although fuel options and combustion technologies are important to analyze on a global or a European level, there are differences in local and regional pre-requisites. Since this is a Swedish pre-study we here choose to present the conditions for the Swedish transportation sector to increase the share of renewable fuels.

Renewable energy for transport

In 2012, the use of renewable energy in the Swedish transport sector amounted to 12.6% when calculated according to the so-called Renewable Energy Directive (RED) calculation rules, i.e., as share of the use of gasoline, diesel, biofuels used in road and rail transport, and electricity in land transport, and with the contribution from biofuels produced from waste, residues, non-food cellulosic material, and ligno-cellulosic material considered double the actual amount (Government Offices of Sweden, 2013; European Parliament and Council, 2009). This was the largest share of renewable fuels for transport among the EU countries (European Commission, 2013) and Sweden will thus meet the target of 10% renewable energy in the transport sector for 2020 stipulated in the RED (unless the use of renewable fuels decreases and/or the energy demand in the transport sector increases substantially or the calculation rules in the RED change).

A domestic biofuel production in the range of 20–35 TWh/year in 2030 seems possible (Börjesson *et al*, 2013; Grahn and Hansson, 2015). The corresponding share of biofuels in the Swedish fuel mix depends on future fuel demand. Grahn and Hansson (2015) elaborate on this uncertainty focusing on two different official fuel demand estimations, generated by Swedish authorities. Fuel demand for road-based transport in Sweden 2030 is projected by the Swedish Energy Agency to 78 TWh/yr (2012a) and by the Swedish Transport Administration to 33 TWh/yr (2012). As a comparison, the current Swedish energy demand for road-based transport is approximately 84 TWh (Swedish Energy Agency, 2012b). The rather different projections come from the different approaches where the Swedish Energy Agency (2012a) represents a long-term prognosis based on current vehicle trends as well as policies, whereas the Swedish Transport Administration (2012) represents a situation in which Sweden focuses on meeting the vision of no net emissions of GHG to the atmosphere by 2050. Depending on estimated demand scenario it can be noted that domestically produced biofuels may either fulfill the entire fuel demand or contribute to less than half of the fuel demand in 2030.

The actual contribution of biofuels for road transport in Sweden in the future will depend on many factors, such as the development of policies (national as well as at the EU level), global developments for fossil fuels and biofuels, the future energy demand, the production and distribution costs for biofuel facilities, the possibility for the Swedish vehicle fleet to use the produced biofuels, and the global competition for biomass and biofuels. There is also the question of public support and willingness of consumers to actually use the biofuels (Sprei, 2013).

Fuel infrastructure and vehicle fleet

The fuel infrastructure and the vehicle fleet may affect the amount of new types of fuels used. The average lifespan for cars in Sweden is around 15 years, meaning that the majority of cars sold today will still be around in 2030, unless incentives are introduced to phase out vehicles at a more rapid pace. Some of the fuel types may be used as blends in conventional fuels, but it is challenging to blend in more than 10–20%, indicating that to meet biofuel shares higher than that, modified vehicles need to enter the market (Grahn and Hansson, 2015).

There are currently 4.3 millions of cars in Sweden and, according to the long-term prognosis presented by the Swedish Energy Agency, the number of cars is projected to increase to around 5.3 and 5.6 millions cars by 2020 and 2030 respectively (Swedish Energy Agency, 2012a; Hansson and Grahn, 2013). The share of cars running on gasoline is projected to decrease from around 3.5 million in 2010 to 2.9 in 2020 and 2.2 million in 2030, whereas the shares of cars fueled with diesel and methane as well as the full electric and hybrid cars are expected to increase. The amount of flex-fuel cars (i.e. cars that can be driven on a mixture of ethanol and gasoline) are projected to remain at around 230 000. Demand from flex-fuel vehicles soared in Sweden between 2004 and 2008, but plummeted after that, due to a combination of lower gasoline prices, changes in subsidies and more fuel efficient diesel vehicles on the market (Sprei, 2013). It can thus be a challenge to create a long term public support and willingness to purchase alternative fueled vehicles.

In 2013, there were in total 2,716 fuel stations in Sweden (SPBI, 2013), the majority offering conventional gasoline and diesel. The number of fuel pumps for alternative fuels has, however, increase over the last decades in Sweden. In 2012, HVO-diesel blends were available at more than 700 locations. There are no technological limitations for the share of HVO that a diesel engine can run on, but most HVO-diesel blends were, in 2012, a mix of 23% HVO and 7% FAME in conventional diesel (Grahn and Hansson, 2015). For methane, DME, and pure FAME fuels, there is some current infrastructure (132, 4, and 22 locations respectively) (SPBI, 2013). An expansion of methane and DME requires a completely new infrastructure to be built. Fuel infrastructure is well developed (1,808 locations) (SPBI, 2013) for the fuel blend E85 (85% ethanol and 15% gasoline) mainly as a result of a Swedish law requiring fuel stations of a certain size to supply at least one renewable fuel. In Sweden, no methanol is currently used in the road transport sector. However, it is possible to blend 3% methanol in gasoline, and adjusted vehicles can run on M85 or M100. The developed E85 infrastructure, gives an advantage to alcohol-based fuels or alcohol blends since it is likely that these pumps and tanks can be flexible and fit also other alcohols than ethanol.

Feedstock and bioenergy supply potential

When studying environmental performance of alternative fuels it is important to know the feedstock used and the production method. Bioenergy is an excellent primary energy source since it contains similar chemical components as conventional oil-based fuels and many types of biofuels can be produced from bioenergy. However, large-scale expansion of biofuel production are also connected to issues such as land-use change, increased food prices, losses in biodiversity and effects on sensitive ecosystems.

Biofuel feedstock

Biofuel feedstock can basically be grouped into four major types (Börjesson *et al*, 2013):

- *sugar-based feedstock*, e.g. sugar cane or sugar beet
- *starch-based feedstock*, e.g. corn, wheat and other cereals
- *oil-based feedstock*, e.g. rape seed, palm oil, tall oil from pulping industry, animal fats from e.g. slaughtering

- *lingo-cellulosic feedstock*, e.g. wood, forest residues, straw, or bagasse.

Algae are another potential feedstock for biofuels with large potential from a long term perspective. With different algae species being built up of different material, a classification according to the above criteria is difficult. However, algae may e.g., be rich of organic carbon which is a good base for anaerobic digestion into biogas or rich of lipids which make them similar to oil-based feedstock.

Bioenergy supply potential

Estimates of global technical bioenergy potentials in 2050 differ by a factor of almost 50 in reviewed literature. Calculations of the potential to grow bioenergy crops on abandoned farmland yielded a potential around 30 EJ/yr (Campbell *et al,* 2008; Field *et al*, 2008), while other studies suggest technical bioenergy potentials of up to 500 EJ/yr (e.g., Dornburg *et al*, 2008, 2010), some even reporting potentials exceeding 1000 EJ/yr (Smeets *et al*, 2007; Ladanai and Vinterbäck, 2009). As Creutzig *et al* (2014), in our review (Heyne *et al, 2015)* we could not find any consensus on the magnitude of the future global technical bioenergy potential, still research has helped to better understand some of its many structural determinants.

Taking into account the risks connected to large scale bioenergy expansions, we agree with many of the authors reviewed in Heyne *et al* (2015) that up to 100 EJ[1] of biomass for energy applications can be produced in a sustainable way and that 300–500 EJ/yr may be technically possible but that such expansion might challenge sustainability criteria. Bioenergy over 500 EJ we find extremely difficult to produce in a sustainable way. Assuming that all of the sustainable produced biomass will be used for the production of biofuels for transport, and accounting for around 50% conversion losses, we find that maximum 50 EJ of sustainable biofuels may be available for the global transportation sector. This can be compared to a currant global demand for transportation fuels of 100 EJ.

For Sweden the biomass potential estimates range between 50 and 85 TWh/yr and up to 100 TWh/yr if a 30–50 year perspective is taken into account (Börjesson *et al*, 2013), which after conversion losses correspond to around half in terms of biofuels, depending on energy conversion technology and the amount of biomass that can be allocated to the transport sector. Depending on estimated demand scenario domestically produced biofuels may either fulfill the entire fuel demand or contribute to less than half of the fuel demand in 2030. For a discussion around this see e.g. Grahn and Hansson (2015) and Börjesson *et al* (2013).

Challenges connected to large-scale expansion of biofuel production

Challenges connected to the agriculture/forestry part of the biofuel system are e.g., the amount of input energy and the emissions of CO_2 arising directly from the soil as well as emissions of methane and nitrous oxide which are 25 and 296 times stronger greenhouse gases than CO_2, respectively. Improvement potentials for emissions reductions within the agriculture/forestry part of the Well-To-Tank (WTT) chain include changing the use of diesel to low-CO_2-emitting fuels, changing to more fuel-efficient tractors, more efficient cultivation and manufacture of fertilizers (commercial nitrogen fertilizer can be produced in plants with nitrous oxide gas cleaning) as well as improved fertilization strategies (more precise nitrogen application during the cropping season). Furthermore, the

[1] These numbers refer to the resource of primary bioenergy, due to conversion losses, the figure would be approximately halved when considering biofuels.

cultivation of annual feedstock crops could be avoided on land rich in carbon, such as peat soils and new agriculture systems could be introduced that lower the demand for ploughing and harrowing (Alvfors *et al*, 2010).

Land-use change (LUC) is an important aspect when assessing the sustainability aspects of biofuels. Changes in land use can result from a wide range of anthropogenic activities including agriculture and forestry management, livestock production and biofuel production. Direct effects of land-use change (dLUC) include changes of carbon stock in standing biomass, biodiversity impacts, nutrient leakage, etc. Beside the direct effects, indirect effects (iLUC) can influence other land uses through market forces across countries and continents. These indirect effects are complex to measure and observe. Increased demand for agriculture or forestry feedstock for the production of biofuels always leads to land use changes, assuming that other agriculture and forestry activities remain. To avoid fertility losses in agricultural soils during biofuel production, crops with low fertilizer needs, high nutrient use efficiency and high yields should be given priority (Höglund *et al*, 2012). In both agriculture and forestry systems great care must be taken to develop sustainable biofuel production.

Another challenge connected to an expansion of biofuel production is the competition with food production resulting in a risk for increased food prices. Several studies show that there is an effect on food prices that can be connected to biofuel expansion. The main question is just how big this effect is. Persson (2014) in a review of studies finds that increase of corn-based ethanol stood for 14–43% of the increase of US corn prices between 2000 and 2008. It has been shown that most households in rural areas are negatively affected from increase food prices in a short term perspective (Bryngelsson *et al*, 2012). A more complex question is how sustained high food prices may affect poverty levels in the longer term (Ivanic and Martin, 2008). Sometimes the suggested solution is to avoid a feedstock that can be used for food as well. However, due to land competition there might still be an effect on food prices regardless of what type of crop that is used for biofuel production. Even using marginal land may not solve the problem if the willingness to pay for biofuels is very high (Bryngelsson & Lindgren, 2013).

The availability of water is, further, a risk factor connected to an increased biofuel production. Freshwater is already scarce in some regions of the world and water demand for bioenergy production might place an additional burden on water availability worldwide. No general conclusions can, however, be drawn from the literature review. It depends on what crop is being replaced and how water intensive the biomass feedstock is. There might be positive effects if drought resistant crops are used (Berndes, 2008). Other studies show that water availability might be a limiting factor for bioenergy potentials (Moldon, 2007; de Fraiture *et al*, 2008; van Vuuren *et al*, 2009; Dornburg *et al*, 2010).

Challenges connected to a globally large-scale expansion of biofuel production may, however, not necessarily apply to an increased biofuel production in Sweden. Advantages for Swedish biofuel production are the large biomass supply potential from forestry residues in combination with Sweden being a sparsely populated country implying no immediate land scarcity. In addition, from a long tradition of pulp and paper industry, Sweden has a well-established infrastructure for handling large volumes of biomass as well as a built out refueling infrastructure for E85.

Fuel production

Apart from sustainability aspects connected to the feedstock it is equally important to study aspects connected to the fuel production, here we focus on biofuels and electrofuels.

Biofuels

The major components in a feedstock basically determine the type of processing that is most adequate for biofuel production. Three major process platforms for biofuel processing exist:

- *thermochemical conversion*, basically biomass gasification, in particular suitable for lignocellulosic material,
- *biochemical conversion* processes (e.g. fermentation, anaerobic digestion) mainly applied to sugar- and starch-based feedstock and
- *hydrogenation/esterification* processes for conversion of oil-based materials, such as vegetable oils or animal fats, to fuels (mainly FAME and HVO).

While being far from a complete mapping of all imaginable processing pathways, Figure 2 illustrates the complexity and variety of major process chains currently discussed.

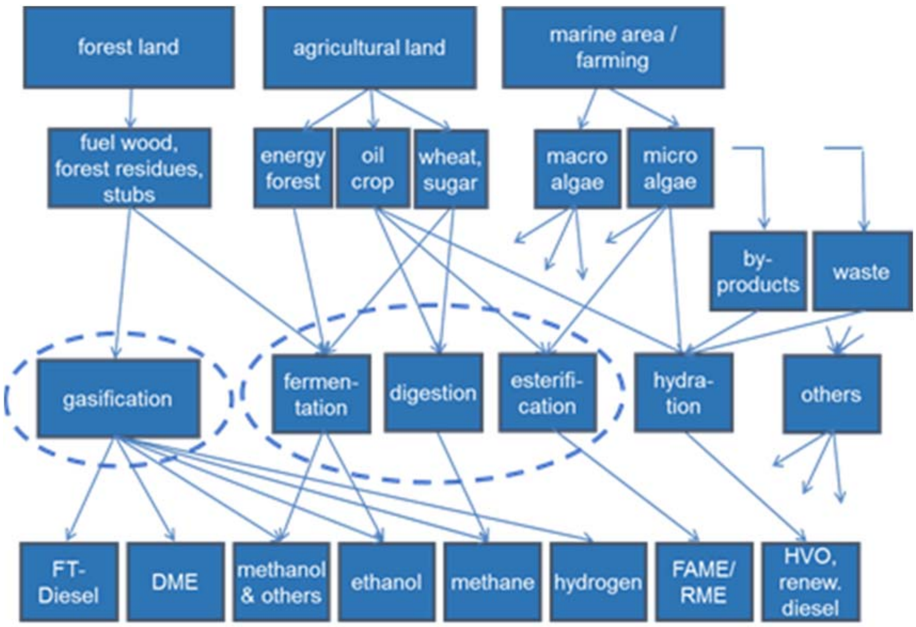

Figure 2. Major production pathways for currently discussed biofuel alternatives (adapted from Börjesson *et al* (2013)).

More details from the literature review on biofuel production can be found in Heyne *et al* (2015).

Electrofuels

Apart from breaking up bindings in biomass to create useful molecules for biofuels it should be noted that hydrocarbons, alcohols and other fuels also can be build up from smaller molecules. One example of this is the production of so called electrofuels. Electrofuels is an umbrella term for carbon based fuels produced with electricity as the main energy source[2]. The carbon content in the fuel may

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[2] Hydrogen, produced via electrolysis, is in theory also an electrofuel. We have, however, chosen to follow the definition used in the comprehensive Swedish governmental investigation FFF, defined in the background report by Nikoleris and Nilsson (2013).

come from carbon dioxide that has been captured from air, seawater, chimney gas, gasification of fossil sources or biomass, or surplus carbon dioxide that is generated in biofuel production facilities. Electrofuels in the form of e-methane, e-methanol and e-DME are the most energy-efficient fuel choices but it is technically possible to convert these molecules to longer carbon chains such as e-gasoline and e-diesel.

Several steps are needed to produce electrofuels (Figure 3): (i) producing hydrogen from water (electrolysis), (ii) capturing CO_2, and (iii) mixing hydrogen and CO_2 to form different types of electrofuels (the Sabatier reaction).

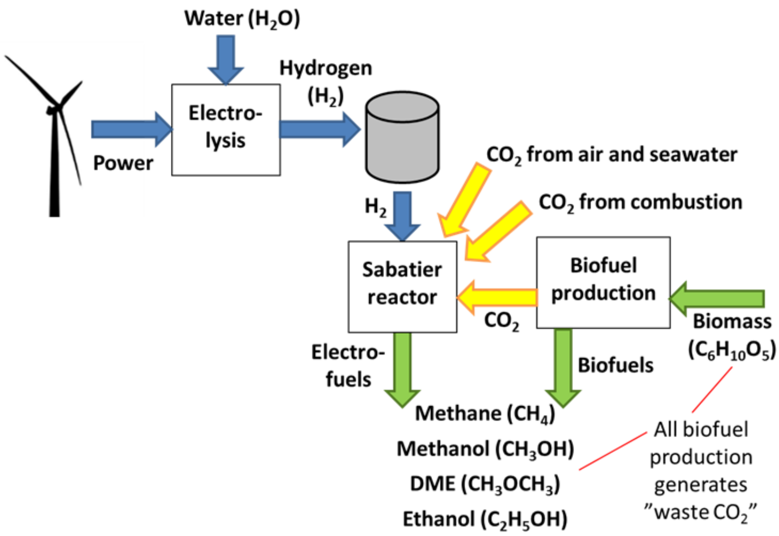

Figure 3. Process steps in the production of electrofuels where the main reaction occurs in the Sabatier reactor where CO_2 and H_2 form different types of electrofuels. The CO_2 can be derived from different carbon sources (Grahn *et al*, 2014).

Current interest in electrofuels from the industry is for example that the shipping company Stena Line sees methanol as a possible replacer of oil[3] and has, as a start, converted one of four engines at Stena Germanica to run on methanol. If the demonstration turns out positive Stena plan to convert 25 of 34 ferries to run on methanol during the next few years and sees e-methanol as a future renewable option. Another example is Audi that has invested in a 6 MW electrofuel plant in Germany that uses wind and solar electricity to produce e-methane[4]. A third example is the Icelandic renewable e-methanol company, Carbon Recycling International[5], that built their first commercial electrofuel plant in 2012 with a capacity to produce more than 5 million liters e-methanol per year for the purpose of blending 3% methanol in gasoline. The CO_2 feedstock and the power for producing electrofuels are both supplied by a geothermal power plant and the electricity price on Iceland is very low.

Grahn *et al* (2014) show that assuming that CO_2 is available free of charge, that the electricity price is not higher than 30 EUR/MWh, and that the oil price is above 100 USD/barrel, e-methanol could be

[3] Ny teknik. Stena Line satsar på metanol. www.nyteknik.se/nyheter/fordon_motor/fartyg/article3667269.ece
[4] Audi e-gas. Energy turnaround in the tank. www.audi.com/content/com/brand/en/vorsprung_durch_technik/content/2013/10/energy-turnaround-in-the-tank.html
[5] Carbon Recycling International (CRI). http://www.carbonrecycling.is/.

profitable, given the production process is running at full capacity at least 45% of the year. Production costs increase significantly only when the process runs less than approximately 15% of the year.

Fuel properties

Conventional fuels are complex mixtures that typically contain more than 100 chemical components. Part of this composition has changed and evolved over time in connection to engine development, in order to meet the developing demand on power, efficiency, driveability and, over the last decades, ever more stringent emissions legislations. When discussing alternatives to current fossil based fuels for propulsion and power generation fuel properties are important criteria from a combustion point of view to take into consideration, since the combustion behavior relates to the main purpose of the heat machine, i.e., to convert chemical power to mechanical power. However, the fuel in an internal combustion engine undergoes other processes and passes many systems before it is burned and these also have to be considered. Here we summarize some of the main fuel properties that should be considered.

Fuel standard specifications are applied to assure that commercially available fuels will achieve engine performance and that the emissions commensurate with the manufacturer's specifications. Standards typically cover four main areas of interest for the engine manufacturers, the society and the customer:

1. Combustion performance (efficiency, power, driveability) and emissions
2. Engine systems influence
3. Transportability (of fuel)
4. Safety and environmental impact

Alternative fuels data center, at the Department of energy in the US, has published a comparison matrix of most commonly discussed alternative fuels and the most relevant information is presented in Table 1 (DOE, 2014).

Table 1. Fuels properties for today's main alternative fuels (DOE, 2014).

	Gaso-line/ E10	Low sulfur Diesel	Biodiesel	Propane (LPG)	Compressed natural gas (CNG)	Liquefied natural gas (LNG)	Ethanol/ E100	Methanol	Hydrogen	Electricity
Chemi-cal stru-cture	C_4 to C_{12} and ethanol ≤10%	C_8 to C_{25}	Methyl esters of C_{12} to C_{22} fatty acids	C_3H_8 majority and C4H10 minority	CH_4 (majority), C_2H_6 and inert gases	CH_4 same as CNG with inert gases <0.5%	CH_3CH_2OH	CH_3OH	H_2	N/A
Feed-stock	Crude Oil	Crude Oil	Fats and oils from e.g. soy beans, waste cooking oil, animal fats, and rapeseed.	A by-product of petroleum refining or natural gas processing	Underground reserves and renewable bioga	Underground reserves and renewable biogas	Corn, grains, agricultural waste, cellulose	Natural gas, coal, woody biomass, waste	Natural gas, methanol, electrolysis of water	Coal, nuclear, natural gas, hydro, wind, solar
Gasoline gallon equivale nt (GGE)	97% - 100%	1 gallon of diesel has 113% of the energy of one gallon of gasoline.	B100 and B20 have 103% and 109% of the energy in one gallon of gasoline and 93% and 99% of the energy of one gallon of diesel, respectively.	1 gallon of propane has 73% of the energy of one gallon of gasoline.	5.66 and 6.38 pounds of CNG have 100% of the energy of one gallon of gasoline and diesel respectively.	5.38 and 6.06 pounds of LNG have 100% of the energy of one gallon of gasoline and diesel, respectively.	1 gallon of E10 and E85 have 96.7% and 73-83% of the energy of one gallon of gasoline (variation due to ethanol content in E85).	1 gallon of methanol has 49% of the energy of one gallon of gasoline.	1 kg of H_2 has 100% of the energy of one gallon of gasoline.	33.7 kWh has 100% of the energy of one gallon of gasoline.
Energy content (lower heating value)	112,114–116,090 Btu/gal (31,3-32,4 MJ/l)	128,488 Btu/gal (35,8 MJ7l)	119,550 Btu/gal for B100 (33,4 MJ/l)	84,250 Btu/gal (23,5 MJ/l)	20,160 Btu/lb (46,9 MJ/kg)	21,240 Btu/lb (49,4 MJ/kg)	76,330 Btu/gal for E100 (21,3 MJ/l)	57,250 Btu/ga (16,0 MJ/l)l	51,585 Btu/lb (120 MJ/kg)	3,414 Btu/kWh
Energy content (higher heating value)	120,388–124,340 Btu/gal (33,6-334,7 MJ/l)	138,490 Btu/gal (38,6 MJ/l)	127,960 Btu/gal for B100 (35,7 MJ/l)	91,420 Btu/gal (25,5 MJ/l)	22,453 Btu/lb (52,2 MJ/kg)	23,726 Btu/lb (55,2 MJ/kg)	84,530 Btu/gal for E100 (23,6 MJ/l)	65,200 Btu/gal (18,2 MJ/l)	61,013 Btu/lb (142 MJ/kg)	3,414 Btu/kWh
Physical state	Liquid	Liquid	Liquid	Pressurized Liquid	Compressed Gas	Cryogenic Liquid	Liquid	Liquid	Compressed Gas or Liquid	Electricity
Cetane number	N/A	40-55	48-65	N/A	N/A	N/A	0-54	N/A	N/A	N/A
Pump octane number	84-93	N/A	N/A	105	120+	120+	110	112	130+	N/A
Flash point	-45°F (-43 °C)	165 °F (74 °C)	212 to 338 °F (100-170 °C)	-100 to -150 °F (-73 to -101 °C)	-300 °F (-184 °C)	-306 °F (-188 °C)	55 °F (13 °C)	52 °F (11 °C)	N/A	N/A
Autoig-nition tempe-rature	495 °F (257 °C)	~600 °F (316 °C)	~300 °F (149 °C)	850 to 950 °F (454-510 °C)	1 004 °F (540 °C)	1 004 °F (540 °C)	793 °F (422 °C)	897 °F (481 °C)	1 050 to 1 080 °F (566-582 °C)	N/A

According to Mauss *et al* (2015) general ideas on fuel properties can be described as depending on: (1) functional groups, such as alcohols, esthers, alkanes, etc; (2) the length of the molecule; and (3) the structure of the molecule, such as straight or branched, aromatic structures, double bonds etc. A comparison on octane numbers (RON), cetane numbers and viscosity connected to the molecule lengths has been presented by Mauss *et al* (2015), see Tables 2–4.

Table 2. Octane numbers (RON) for some carbon based fuels of different molecule lengths (Mauss *et al*, 2015).

	C_1	C_2	C_3	C_4	C_5	C_6	C_7	C_8	C_9	C_{10}
Alkanes	120	108	105	93	62	25	0	-20		
Alkenes (A)						76	66			
Alcohols (B)	109	109	105	96	85	59				
Aromatic (ring)						101 (C)				90 (D)
Aromatic (Methyl group)							120 (E)	118 (F)		
Ether (centered O)		35		0						

(A) Referring to double bond on the first position. (B) Alcohol group on the first position, e.g., 1-butanol. (C) Benzene. (D) Naphthalene. (E) Toluene. (F) Xylene.

Table 3. Cetane numbers for some carbon based fuels of different molecule lengths (Mauss *et al*, 2015).

	C_8	C_{10}	C_{12}	C_{14}	C_{16}	C_{18}	C_{20}
Methyl esters	33.6	47.2	61.4	67.0	74.5	86.9	
Alkanes (A)	63.8	76.9	87.0	96.3	100	108	112

Table 4. Viscosity expressed as micro Pascal seconds at 20 ^oC for some carbon based fuels of different molecule lengths (Mauss *et al*, 2015).

	C_1	C_2	C_3	C_4	C_5	C_6	C_7	C_8	C_9	C_{10}	C_{12}
Alkanes					222	320	410	530	710	920	1500
Alcohols	610	1190	1900	2900							
Aromatic (ring)						610 (A)				2400 (B)	
Aromatic (Methyl group)							590 (C)	620 (D)			

(A) Benzene. (B) Naphthalene. (C) Toluene. (D) Xylene.

Mauss *et al* (2015) also present a rule of thumb for liquid and solid fuels when it comes to calculate the energy content (in lower heating values - LHV) of a fuel that contains the atoms carbon, hydrogen and oxygen:

$$\text{Energy content LHV [MJ/kg]} = 32.8 \times m(C) + 101.6 \times m(H) - 9.8 \times m(O)$$

and two examples of using the formula are: (1) n-Heptane = 26.9 + 18.1 – 0.0 = 45 MJ/kg, and (2) n-Hexanol = 23.3 + 14.2 – 1.5 = 36 MJ/kg.

Heat of vaporization is, further, an important property to take into account when trying to identify good fuel candidates. Higher heat of vaporization improves knock resistance and enables achieving higher engine efficiency, but may also lead to problems related to start up and to run a cold engine (Wallner *et al*, 2012). Heat of vaporization is substantially higher for ethanol than for gasoline (see Figure 4), while heat of vaporization of longer chain alcohols, such as butanol isomers, is closer to that of gasoline (and since gasoline contains both olefins and paraffins it can be approximated as the blue line in Figure 4).

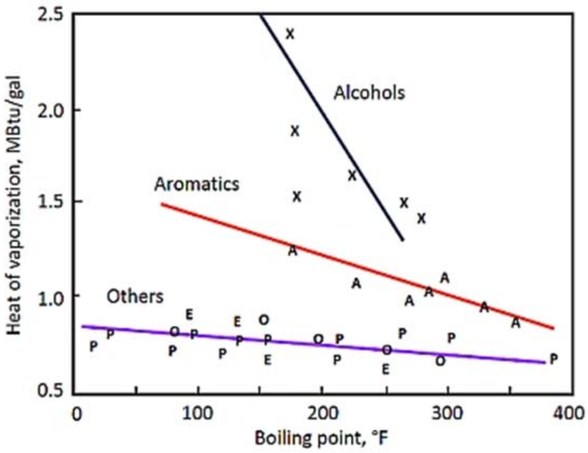

Figure 4. Heat of vaporization for alcohols, aromatics, olefins (O), paraffins (P), and ethers (E) (Piel and Thomas, 1990). Note that °C=(°F-32)/1.8.

Flame temperature is another important property that may guide towards good fuel candidates. Flame temperatures of some alcohols are lower[6] than those of e.g. aromatics, see Figure 5. However, if alcohols lead to leaning of air to fuel ratio (indicate a possible surplus of oxygen), combustion temperature rises (Piel and Thomas, 1990). Flame temperatures for butanol are close to those of gasoline (and since gasoline contains both olefins and paraffins it can be approximated as the blue line in Figure 5).

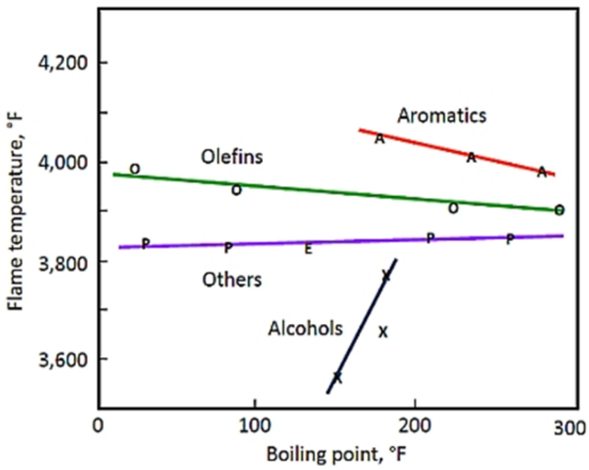

Figure 5. Theoretical flame temperatures for alcohols (X), aromatics (A), olefins (O), paraffins (P), and ethers (E) assuming adiabatic process and stoichiometric air to fuel ratio (Piel and Thomas, 1990). Note that °C=(°F-32)/1.8.

Not mentioned in the above comparisons but promising fuels, similar to conventional diesel and increasingly investigated over the last years (Machado, 2013; Hamilton, 2014), into straight or branched olefin hydrocarbon chains called farnesenes, derived from the fermentation of sugar or cellulose. The olefin is further treated in a hydration step, removing double bounds, into a branched alkane. These hydrocarbons, with chain lengths of ~C15 show properties directly comparable to

[6] A lower flame temperature tends to lower NOx emissions but increase emissions of unburned hydrocarbons.

diesel without further additives. Heating value on a mass base is slightly higher for farnesenes compared to diesel, but since density is slightly lower the resulting energy per volume base is similar to conventional diesel. The viscosity is within the specification range for diesel which promises good operation in pump- and injection system. Boiling and distillation indicates a slightly flatter distillation curve, but not higher final temperature which is important to spray and flame formation. A slightly higher 10% distillation temperature indicates a higher initial boiling point which might influence oil dilution (compare with FAME). In engine testing, the fuel was tested as blend with diesel and as neat 100% fuel (Machado, 2013; Hamilton, 2014). The results on engine performance were promising with minor effects on efficiency and power, and with a reduction of measured emissions. The presented studies on these fuels have to current knowledge been focused on engine operation in controlled conditions while the stability parameters such as oxidations stability and low temperature performance, CFPP (Cold filter plugging point) and cloud point, are not presented.

More details from the literature review on fuel properties can be found in Holmborn (2015).

Health effects of fuels

Several studies indicate that alternative fuels like RME, DME, methanol, ethanol and methane can have health, safety and environmental benefits compared to gasoline and diesel. Ahlvik *et al* (1999) give a good overview and include results that show that alternative fuels reduce the risk for cancer. Later studies on particles negative health effects further reinforce these results. Other studies such as Ginnebaugh *et al* (2010) show that, especially in cold weather, ethanol may increase the formation of ozone and that emissions of acetaldehyde and formaldehyde, which both are considered carcinogens, might be higher. The US Environmental Protection Agency draw the conclusion that a shift from gasoline to methanol would reduce the risk of fires and explosions with 95% (Machiele, 1990), while Ahlvik (2002) gives several examples where methanol spills would have a substantially lower environmental impact than oil spills. As an example of this, none of the experts that were called to examine a spill of 80,000 liters of methanol in the Rhine could find any long-term effects. However, methanol is a controversial fuel due to its high toxicity and thus has to be handled carefully if introduced as a fuel. There is however a long experience considering methanol to be a widely used base chemical.

Engine performance

A wide range of alternative fuels have been tested in internal combustion engines and from the literature review an overview of technical issues, potential engine efficiency and emissions have been identified (Tunér, 2015). Different fuels may perform differently depending on type of combustion engine and therefore have different environmental impact.

Engine concepts

The two most common engine concepts are the spark Ignition (SI) and the compression ignition (CI) engines where the most relevant advantages and disadvantages are presented in Figure 6.

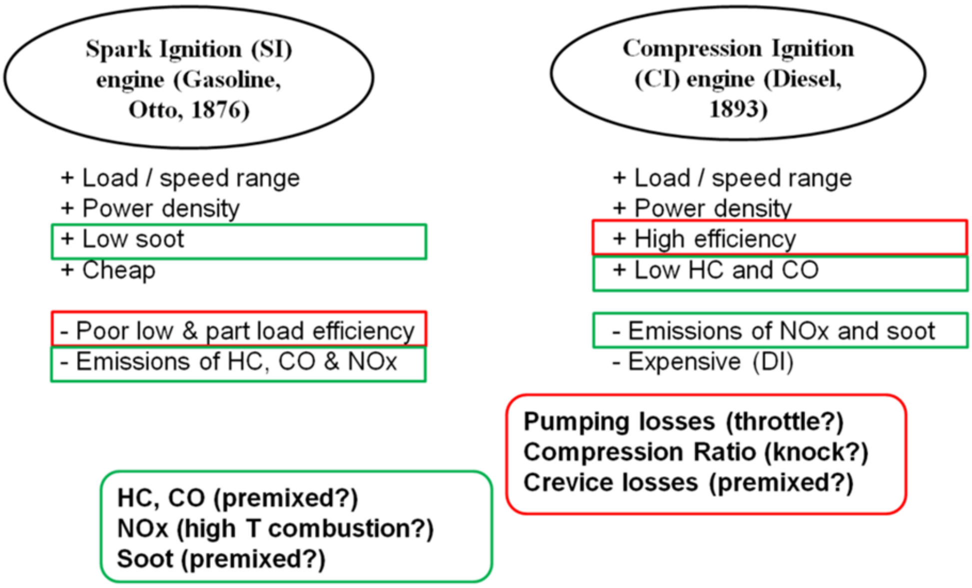

Figure 6. Overview of some advantages and disadvantages of spark ignition (SI) and compression ignition (CI) engines. Red boxes are related to efficiency while green boxes are related to emissions. The question marks connected to "premixed" indicate the uncertainties around that premixing (typical for SI) leads to fuel becoming trapped in crevices and give raise to higher emissions of HC and CO. The premixing reduces, however the risk of fuel rich zones and thus soot emissions. SI is throttle controlled and this leads to increased pumping losses. SI is also knock sensitive, which is avoided with limited compression ratio.

Apart from SI and CI other combustion concepts are being researched in order to find more efficient and clean combustion principles. Homogeneous charge compression ignition (HCCI) is a low temperature combustion strategy that over the years has given insights that has led to the development of many other concepts, including Reactivity controlled compression ignition (RCCI) and partially premixed combustion (PPC).

A common feature of the new combustion principles is that they offer new opportunities for both existing and new alternative fuels. HCCI can be run on essentially any fuel by tailoring compression ratio and inlet temperature, RCCI uses two fuels with varying proportions while PPC runs efficiently on any liquid fuel by adjusting fuel injection and other parameters. PPC has also demonstrated excellent efficiency and very low emissions for naphtha, that has an octane rating of around 70; essentially a fuel with ignition properties in-between diesel and gasoline. An illustration of how the new engine concept PPC and RCCI relate to conventional SI and Direct Injection Compression Ignition (DICI) engine concepts, regarding how suitable the engine concepts are to reactive fuels like diesel and none-reactive fuels like gasoline, can be seen in Figure 7.

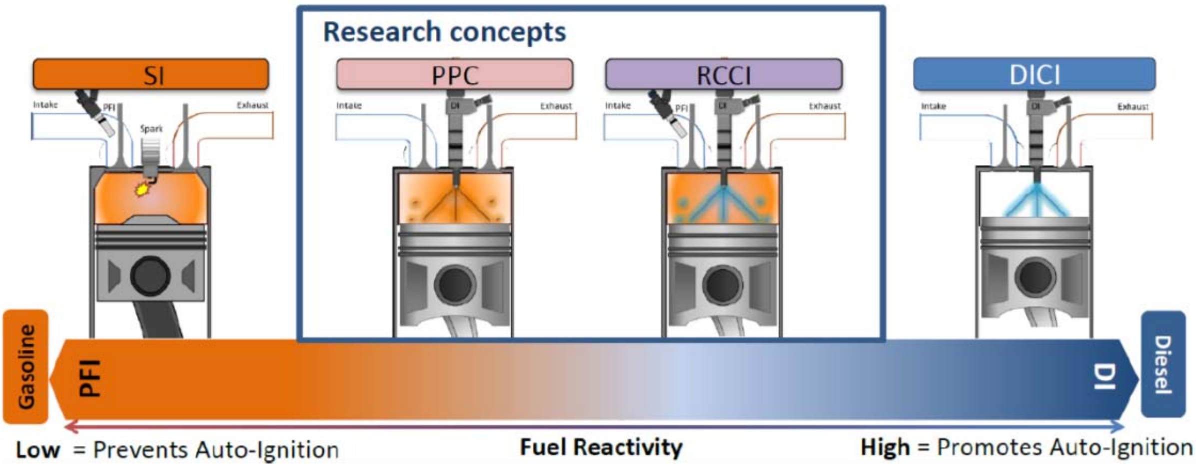

Figure 7. Engine combustion research concepts compared to conventional spark ignition (SI) and Direct Injection Compression Ignition (DICI). Blue indicates a reactive fuel like diesel while orange indicates a none-reactive fuel like gasoline. Modified from Curran *et al* (2012).

Efficiencies and emissions

According to Mauss *et al* (2015) the following general conclusion can be drawn regarding soot and NOx formation from combustion of alternative fuels.

- Formation of soot depends strongly on the structure of the molecule and a general trend is that: Alcohols < Esther < n-Alkanes < iso-Alkane < n-/iso Alkenes < Aromats/Cyclic fuels, where alcohols are the best choice in terms of soot formation.
- Formation of NOx depends on the combustion process, and not only on the selected fuel, where a strong relation is connected to the in-cylinder temperature, where lower temperature produces less NOx.

From the literature review (Tunér, 2015) relevant data and combustion results on soot emissions and energy efficiency for different fuels in different engine combustion concepts are summarized in Figures 8–9. A summation and comparison on HC, CO, and NOx emissions can be found in Tunér (2015). Since the data set is limited, the influence from different individual engine operation conditions can be such that the presented results are not always directly comparable meaning that these figures should be regarded as indications rather than universal truths. All emissions data are engine-out emissions, thus before any emissions after-treatment system.

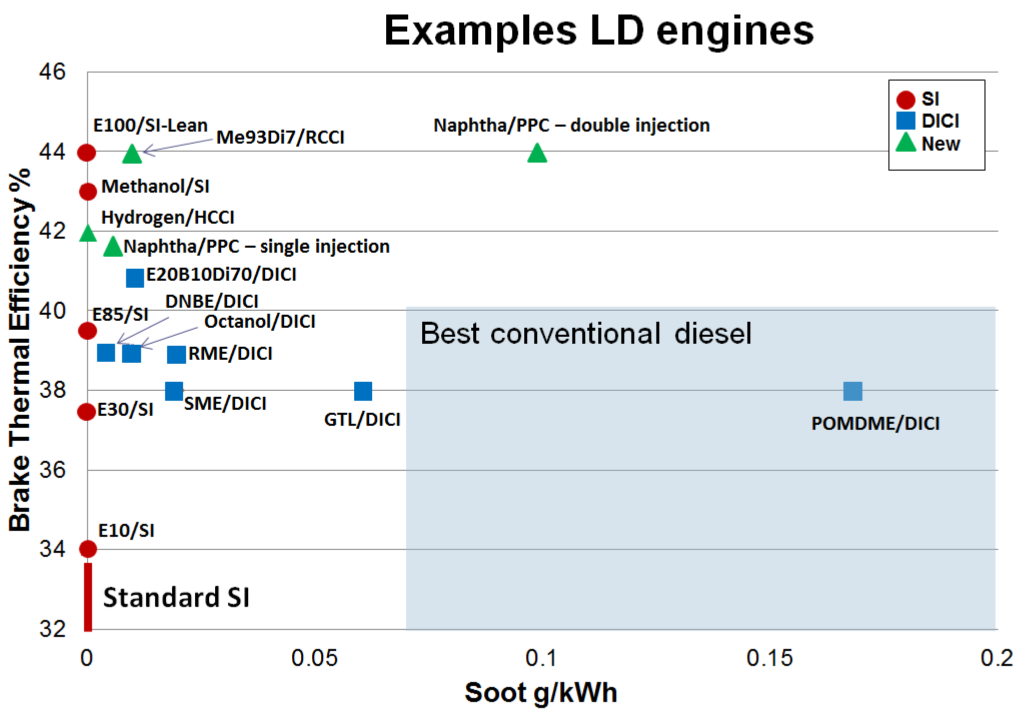

Figure 8. Soot emissions and brake thermal efficiency for different fuels and light-duty (LD) engine combustion concepts.

In Figure 8, one can see that going from current commercial gasoline with 5% ethanol to neat ethanol, efficiency can be increased by a remarkable 30% thanks to beneficial evaporation properties and the allowed increase in compression ratio due to the higher resistance against knock plus lean operation. Methanol allows as well for very high efficiencies and low soot emissions. The high molecular expansion (the so called mole factor = 1.17) of methanol should in theory lead to an efficiency advantage over ethanol. Figure 8 also shows that alcohols in SI do provide a significant benefit compared to gasoline and even surpasses diesel engine efficiency combined with essentially soot free operation. Alternative diesel-like fuels such as rapeseed methyl ester (RME), soy methyl ester (SME) and gas to liquid (GTL) provides important soot reduction but do not alter efficiency. The results on POMDME are not characteristic for DME-like fuels and are likely an effect from a less than ideal combination of operating parameters and hardware. The same set of experiments provided even much worse performance for fossil diesel fuel. POMDME is known to produce lower soot, HC and CO than diesel.

The emerging combustion concepts such as HCCI, RCCI and PPC provide high efficiencies and comparably low soot emissions. Naphtha/PPC with double injection showed higher efficiency but also quite high soot compared to single injection.

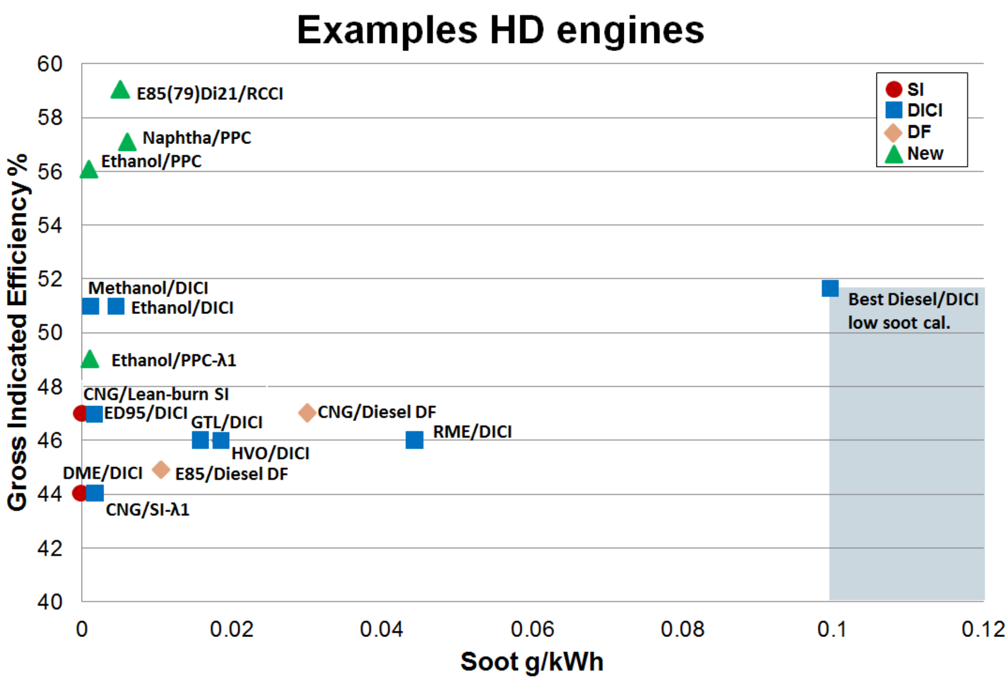

Figure 9. Soot emissions and gross indicated efficiency (GIE) for different fuel and heavy-duty (HD) engine combustion concepts.

Figure 9 reveals that most alternative fuels have an advantage compared to fossil diesel regarding soot emissions. Just as for LD engines, the alcohols show a strong advantage. There are some variations in gross indicated efficiency (GIE) between fuels using the DICI principle, but this is mainly an effect of using different hardware or operating conditions. Alternative liquid fuels, such as synthetic diesel (GTL), HVO or RME should in principle have the potential to reach similar peak efficiency as the state-of-the-art DICI engine included in Figure 9. This engine has 51.6% GIE and 47.0% brake thermal efficiency (BTE). There are essentially no combustion losses, while pumping losses are 1.6% and friction losses are 3.0% and thus represent the drop from BTE to GIE of 4.7% from the used 100% fuel energy. PPC is expected to have a larger drop in efficiency down to 48–50% BTE while the loss might be even bigger for RCCI due to the use of extensive Miller timing[7] and high boosting requirements.

The DICI engine running on neat ethanol or methanol is actually a medium duty engine showing good potential for efficiency and soot. The indicated efficiency estimated in Roberts, Johnson and Edwards (2014) is based on the assumption of turbo-compound. The largest stationary CNG/SI engines, used for production of electricity, exhibits GIE above 55% while their smaller contemporary truck engines shown in Figure 9 have more modest efficiencies. Soot is essentially none-existent. Dual-fuel engines with diesel pilot produce soot from the diesel fuel and in the case of CNG show diesel-like efficiency. The E85/diesel dual fuel engine has slightly lower efficiency and very high emissions of HC, CO and NOx. The reason is likely related to the yet limited amount of research spent on this concept. Soot is low though. The new combustion concepts RCCI and PPC show substantially higher efficiencies and lower soot levels.

[7] With Miller timing the effective compression stroke is shorter than the expansion stroke. Almost all engines today employ mild Miller timing since it is usually good for thermodynamic efficiency. More excessive Miller timing require very efficient boost systems to be beneficial.

More details from the literature review on engine performance can be found in Tunér (2015).

Well-to-wheel and system studies of fuels

When evaluating biofuels from a sustainability perspective all three dimensions of sustainability, i.e., environmental, economic and social should be taken into account. This is challenging, especially taking into consideration the social perspective that is often less quantifiable. Indicators that cover all or some of the above mentioned dimensions have to be set. Obviously, on a general level, these indicators can be defined in numerous ways with considerable differences for example between studies having a life cycle assessment (LCA) perspective and studies focusing on industrial systems analysis, according to Börjesson *et al* (2013). The definition of the systems boundaries can, in addition, have a large impact on the actual value of the different criteria. Thus, a very important aspect for enabling a transparent comparison between different studies is the proper definition of systems boundaries and how cogenerated by-products are valued. Other aspects that are important to take into consideration are: how feedback loops are handled, if the modeling is general or location specific, how uncertainties are handled (in a deterministic or stochastic way) and the time horizon used.

A number of studies have been investigating the whole value chain from well to wheel, meaning from the extraction (or growth) of primary energy sources (well) through the energy conversion processes and different transportation steps to the end-use in passenger cars or trucks (wheel), with focus on illustrating different perspectives on performance and ranking among fuels. Studies are performed either by industrial consortia or institutions (e.g., Volvo, 2008; E4tech, 2013; Albrecht *et al*, 2013; ERTRAC, 2014; Edwards *et al*, 2014) or by scientific committees (e.g., KVA–Energiutskottet 2013; EASAC, 2012). These studies compare various fuels based on different criteria where the two most common are climate impact and energy efficiency, but also other criteria such as fuel costs, feedstock potential, distribution infrastructure, and other economic, environmental and societal sustainability issues may be assessed.

The JEC well to wheel study (Edwards *et al*, 2014) stresses the increased energy use for alternative fuels in relation to fossil fuels. They also point out that the greenhouse gas emission performance in relation to standard fossil fuels is strongly dependent on the combination of production pathway and powertrain alternative. Both cost and GHG emission results are presented in the report of the German Research Association for Combustion Engines (FVV) (Albrecht *et al,* 2013) with costs (without taxes) for biofuel alternatives ranging between 2.8 and 6.7 $€/l_{Diesel\text{-}equivalent}$ against a reference price range for fossil fuel of 0.64 to 1.18 $€/l_{Diesel\text{-}equivalent}$. Biofuels are stated to have the potential to almost completely avoid the GHG emissions from fossil fuels (about 90 g CO_2-eq/MJ) but at rather high avoidance costs ranging from about 500 to 1400 €/t CO_2-eq avoided.

The systems studies presented in Heyne *et al* (2015) all have adopted a somewhat different analysis approach, made different assumptions and come up with different results. Here we present a summary of these studies highlighting where they have common conclusions and where there are conflicting views. Some of the systems studies, especially if analyzing a short term perspective between 2020 and 2030, highlight the possibility of increasing the use of renewable fuels through higher shares of blend-in levels of renewable fuels, or additives, to today's major fuels, i.e. diesel and gasoline. Increasing the blend-in level to 20% ethanol in gasoline may, however, face challenges where for example the E4tech study concludes that transition to E20 is more likely to be limited by the vehicle fleet transition rather than the sustainable supply of biofuels (E4tech, 2013).

Liquid fuels are clearly in focus for all studies. This again is related to the time horizon the studies have adopted. HVO and FAME are the major biofuels identified as diesel substitutes, whereas ethanol, methanol, butanol[8], ETBE and MTBE are possible blend-in (or even substitute in case of alcohols) alternatives for gasoline. According to the latest version of the EU fuel quality directive (European Commission, 2012) upper limits for blending in FAME fuels in diesel is 7% (former 5%). In the same directive also upper limits are set for ethanol and methanol blends in gasoline to 10% (former 5%) and 3% respectively. Methanol is discussed in the different studies with contradicting results: in the Volvo study (Volvo, 2008) with focus on heavy duty engines methanol scores quite well within all categories whereas for example the FVV study is skeptical about methanol, in particular due to its toxicity (Albrecht *et al*, 2013). The JEC study does not consider methanol as an alternative fuel for engines at all within their timeframe (2020+) and only analyses the well-to-tank aspects (Edwards *et al*, 2014).

Gaseous fuels are identified as very interesting alternatives considering the production processes. In particular biogas from digestion of waste streams performs very well with respect to greenhouse gas benefits (assuming zero or low leakages of methane). Drawbacks for gaseous fuels – renewable methane (or biogas) being the major option – are: the lacking distribution infrastructure, vehicle fleet and, to some extent, the limited feedstock potential (in particular for biogas from household and agriculture waste via anaerobic digestion).

Studies extending the timeframe consider algae-based fuels as interesting options, however, big question marks in particular on feedstock availability and costs remain. Electrofuels are seen as a competitive/complementary alternative to electromobility and their interrelation with renewable electricity generation might be very well adapted to future energy markets. But higher costs and a penalty on efficiency due to conversion steps limit their potential in the short to medium term.

From the range of systems studies reviewed it can be noted that there is no single fuel identified as winning alternative, but that the different fuel options all have possibilities and challenges. Fuels that can be blended into conventional fuels are generally seen advantageous, as well as fuels that can be produced from waste streams or locally available bioenergy sources. For Sweden, fuels based on forestry residues are seen as promising options. Taking these insights into account it is likely that a mixture of alternative fuels will enter the fuel market.

More details from the literature review environmental effects and consequences from a systems perspective can be found in Heyne *et al* (2015).

[8] Note that butanol is also possible to blend with diesel.

Lessons learned from the work at Aachen University

Since 2007 a cluster of excellence[9] at RWTH Aachen University has been working on the development of tailor-made fuels from biomass (TMFB, 2015). In an interdisciplinary approach, more than 70 scientists, funded by the German government, are engaged in analyzing, understanding and optimizing the synthesis and combustion of these fuels. The idea is to be able to create principals and models for fuel design that optimize both biofuel production as well as biofuel combustion. It contains both a model based description of fuel synthesis and production routes as well as specification of targeted fuel properties. There are two integrated research fields. The first one is from biomass to biofuels. In this case the focus has been at what fractions can be extruded from lingo-cellulose. Different conversion processes are then looked at and a set of chosen fuels produced. The second integrated research field is from biofuels to propulsion. This field looks at the integration between combustion kinetics, fuel injection and combustion systems as well as fuel spray, flow and mixing. The fundamental idea is to have a high degree of freedom in the definition of new fuel candidates that at the same time satisfies properties concerning: density, viscosity, compressibility, surface tension, boiling curve, heat of vaporization, ignition delay, burning velocity, heating value and molecular structure.

The cluster of excellence is carrying out research with a systematic approach trying to analyze as many fuel options as possible that can be tailor-made from ligno-cellulose, i.e., the molecules glucose, xylose, and lignin. The relatively long molecules are first cut up in shorter molecule structures containing carbon, oxygen and hydrogen (e.g., levulinic acid and itaconic acid) and thereafter formed into fuels. The process follows five steps from lingo-cellulose to fuel: extrusion, multiphase catalytic extraction, enzymatic depolymerisation, integrated fermentation and selective catalytic transformation. The fuels chosen are all mathematically feasible $C_xH_yO_z$ structures based on the valence rules. Fuels are for example alkanes, alkenes, alcohols as well as more advanced molecules, in all possible carbon lengths and structures (straight or branched, double bonds etc.). The fuels are analyzed from criteria such as accessibility score, reaction yield and life-cycle analysis.

So far the research cluster in Aachen has gathered information from 12,400,000 different molecules in a database. These molecules have then been evaluated from criteria such as having a heating value larger than 30 MJ/kg, an enthalpy of vaporization less than 60 $kJ/kg_{air,\lambda=1}$, a boiling point between 50–100 ºC, and a low auto-ignition tendency, leading to that 279 molecular structures were detected more interesting than the others. Molecules that Aachen presents as promising fuel candidates for the SI engine, among these 279 molecular structures, are e.g., alcohols, aldehydes, ketones, acyclic ethers, acetals, furans, and pyranes, where they currently put most focus on 2-butanone and 2-methylfuran. General conclusions so far is that it is challenging to find something better than alcohols, but that 2-butanone seems to have similar properties as ethanol but perform slightly better at cold starts. Further, 1-octanol seems to be a promising candidate with slightly less soot emissions compared to diesel.

[9] The Excellence Cluster involves more than 20 RWTH departments working in the fields of chemistry, bio-technology, process engineering, and mechanical engineering. It is supported by partner institutions, such as the Fraunhofer Institute for Molecular Biology and Applied Ecology (Aachen) and the Max-Planck-Institut für Kohlenforschung (Mülheim).

Although this thorough systematic approach, Aachen, have not prioritized to analyze fuel blends nor how well the fuels would perform in future engine concepts as PPC and RCCI. They have neither had any close contacts with the automotive industry guiding them in relevance matters. We feel convinced that the knowledge within RWTH Aachen University can be a fruitful complement to knowledge within the Swedish Internal Combustion Engine Consortium (SICEC) where the focus over the years has been on relevant fuel options and blends for the automotive industry. We see possibilities for future productive collaborations.

Discussion and conclusion

In this section we summarize and reflect on results from the literature review focusing on engine related issues, list the most clearly identified conclusions and present identified knowledge gaps indicating need for further research.

Attractive fuel options for combustion concepts in a short term perspective

The presented engine research shows that SI engines work even better on alcohols than on gasoline if efficiency and emissions are accounted. Both peak efficiency and part load efficiency for methanol-SI even surpasses that of diesel engines. Emissions can be ultra-low with three way catalytic converter (TWC) and stoichiometric alcohol operation. Negative aspects are cold start performance, corrosion issues and increased volumetric fuel consumption due to the lower energy content of alcohols. To solve the cold starting issues alcohols are currently not used neat in Sweden, but as ethanol in mixture with gasoline, i.e., E85.

Gasoline fuel is a mixture of hundreds of components that together give a spread in evaporation and ignition properties that are beneficial for cold starting and controlling combustion rate. Similar beneficial properties can be achieved by combining several bio-based hydrocarbons as for instance in ternary blends. The basic idea of the concept of ternary blends enables very interesting opportunities for continuous fuel reformulation without any requirements on updates either to the vehicle or to the fuel distribution infrastructure. By introducing methanol to E85 a larger biofuel base can be exploited and both ethanol and methanol effectively employed with little or no negative impact on SI engine technology. Considering the several positive qualities of alcohols combined with the experiences of E85 and the currently existing distribution system of E85, the concept of ternary blends of gasoline, ethanol and methanol seems very attractive.

On the DICI engine side HVO as well as alcohol mixtures seem the most relevant ones to investigate further in the short term perspective. HVO is an excellent fuel that can be used directly in DICI engines. From an engine performance point of view HVO is better than FAME and since both use the same feedstock research should possibly be directed towards HVO. HVO is, however, currently more expensive than FAME and has worse performance when it comes to biodegradability in case of spillage. Alcohols can be used in DICI engines but require quite other engine specifications and are thus not directly exchangeable with diesel.

For the short term future it seems relevant to focus on alternative fuels that can be used in SI or DICI engines. A plausible path is to increase the amount of drop-in fuels in gasoline and diesel to eventually phase out the fossil fuels in the mixtures.

Attractive fuel options for combustion concepts in a long term perspective

There is still a research need for finding better ignition improvers and possibly the use of alcohols in light-duty DICI engines. If the current trend with lower compression ratio continues for DICI this will require fuels with higher cetane number (McCormick, 2014). POMDME and its derivatives are candidates that at least theoretically could be good for clean DICI operation. Further research is needed though to learn more about how POMDME behave in different combustion conditions. Ternary blends are also relevant for DICI where a baseline specification should be sought and investigated. Ongoing, not yet published work at Chalmers University investigates the performance in DICI with blends of diesel, HVO and n-butanol (Munch, 2014).

Several of the non-commercial alternative fuels have only been investigated to a limited extent, so much more research is required. Many of these fuel components could provide further benefits if mixed with each other or with more well-known alternative components. For instance could a mixture of octanol and di-n-buthyl ether (DNBE) possibly provide good results in DICI.

With the emerging engine combustion technologies there is an opportunity to adapt both fuels and engines to each other. One such opportunity would be to find alternative fuels and blends that can be matched with PPC engine adaption. For instance, it would be relevant to find and investigate alternative fuels with properties similar to those of naphtha – a fuel with combustion properties somewhere in-between gasoline and diesel.

From research carried out at RWTH Aachen University results point towards that 2-butanone and 1-octanol may be a promising future fuel candidates. From the systems studies perspective no single fuel is identified as winning alternative. Fuels that can be blended into conventional fuels are generally seen advantageous, as well as fuels that can be produced from waste streams or locally available bioenergy sources. For Sweden, fuels based on forestry residues are seen as promising options.

Other engine related challenges connected to the use of new fuels

In this literature review, the main focus has been on challenges connected to the combustion of alternative fuels regarding efficiency and most common emissions. Other challenges that may appear could be related to corrosion issues, fuel injection issues and ignition related issues. The emissions after-treatment systems (EATS) will also be facing challenges with new emission components. New fuels may produce specific components in the exhaust stream that are either toxic, cancerogenic or otherwise unwanted. Ethanol, may for example increase the formation of acetaldehyde and formaldehyde, in cold weather, both considered carcinogens. These new emission components could become a challenge to remove with an EATS, since the development towards more efficient engines typically reduces exhaust temperatures that are needed for effective catalytic conversion. Emerging and stricter emissions legislation may pose further challenges, not only on the EATS and the engine system, but also on the fuel.

Conclusions

In this synthesis report we can list the following conclusions.

Conclusions related to the combustion in general

- Internal combustion engines can be adapted to a wide range of fuels.
- Efficiency and emissions performance does not need to be degraded compared to currently existing commercial engine concepts. In fact, efficiencies can be increased substantially with alcohol use in SI engines, which is the most common engine solution today for passenger cars globally.
- The SI principle leads, in general, to low emissions of soot but high emissions of NOx, HC and CO. These are on the other hand treated effectively with three way catalyst (TWC) after-treatment.
- The DICI principle provides low CO and HC but suffers from high NOx and especially soot emissions, which poses some challenges of cost effective and efficient combination of EATS.
- Alternative fuels, that can replace fossil diesel, such as FAME, HVO or alcohols do all show strong reduction of engine-out soot and can be exploited for simplified and cheap EATS.
- The emerging combustion concepts HCCI, RCCI and PPC demonstrate both higher efficiency and lower emissions than conventional SI or DICI. These concepts do also provide emission benefits when operated on alternative fuels.

Conclusions related to how to identify good fuel candidates, from a combustion perspective:

- If the fuel has oxygen integrated in the molecule it tends to decrease soot formation in the combustion, i.e., alcohols and ethers are good fuel candidates from this perspective.
- A fuel with high volatility, and low boiling point, is beneficial since it leads to rapid spray brake-up and mixing. However, important to understand the challenges that come with a fuel with really low boiling point, where for example LNG and DME face challenges from a fuel tank storage perspective.
- To avoid large fuel tanks it is beneficial with a fuel that doesn’t have too low heating value.

Specific aspects when identifying fuel candidates intended for Diesel combustion concept

- The fuel may have a relatively low cetane number, which leads to a delayed ignition and in turn to lower emissions and higher efficiency. It is, however, important that the cetane number is high enough (at least 30) to avoid difficulties with cold starts.
- A low concentration of aromatics is beneficial since they tend to increase emissions of particulate matters.
- In a short-term perspective it is beneficial if the alternative fuel could be blended with conventional diesel and remains within the defined EN 590 standard.

Identified promising fuel candidates

- Alcohols in the range C_1–C_{10} seem promising. Of these ethanol is already a commercial fuel for transport and methanol a common fuel in racing sports.
- Ethers, especially di-n-butylether (DNBE) and POMDME ($CH_3O(CH_2O)nCH_3$) seem promising. These fuels are similar to DME (CH_3OCH_3) with low emissions of soot and NOx but with the

advantage of being liquids that can be blended with e.g., diesel and probably also with alcohols.

- Farnesenes, in either straight or branched olefin hydrocarbon chains, seem promising for use in diesel engines.
- Other emerging candidates such as levulinate and furoate could be important as blend components.
- From the work at Aachen promising options seem to be 2-butanone and alcohols where they highlight the advantages connected to 1-octanol.
- Ternary blends of gasoline, ethanol and methanol can be used in conventional combustion engines and the existing distribution system for E85. They also seem to improve cold start issues compared to just ethanol.

Conclusions related to environmental effects and systems perspectives:

- From a production cost perspective it is beneficial if the fuel either (1) is a small molecule that can be synthesized from syngas or similar processes or (2) a molecule that is similar to molecules in biomass or (3) already is a large scale produced chemical.
- There is no single fuel identified as winning alternative, but different fuel options have possibilities and challenges.
- It is likely that a mixture of alternative fuels will enter the fuel market.
- Regarding how much biofuels that can be produced in a sustainable way we find that maximum 50 EJ of sustainable biofuels may be available for the global transportation sector. This can be compared to a currant global demand for transportation fuels of 100 EJ.
- For Sweden, the biomass supply potential limits the biofuel production to 20–35 TWh/year, which is around a third of current fuel demand.

Identified knowledge gaps and suggested topics for further research

From the literature review we have identified the following research topics where improved knowledge would be beneficial when identifying excellent alternative transportation fuels.

Fundamental understanding of fuel properties

Improved fundamental understanding of fuel properties is essential for the research and development of clean and efficient engines. The current methods and standard tools are to some extent insufficient to provide such understanding or meaningful comparisons of fuels in different combustion strategies, and should therefore be complemented and developed further.

Understand changes in fuel performance

Improved scientific understanding is needed regarding how fuels' properties change depending on engine load. There is also a need to identify fuel candidates that would be excellent choices for the PPC combustion concept, i.e., behave as diesel on low loads and as gasoline on high loads.

Ternary blends

Further development of the concept of ternary blends, to achieve high fractions of alternative fuels without upsetting engine calibration or functionality of control systems or EATS in SI and DICI, could be relevant to investigate further.

Storage, distribution, handling, and health effects

Studies of storage, distribution and handling as well as health effects of new fuels are limited. We have also identified knowledge gaps around favorable blending proportions and the different blend's effects on fuel systems including engine components.

System perspective studies

Knowledge gaps related to systems perspectives are summarized in Figure 10 qualitatively showing the state of knowledge (green shading) and the research need (question mark symbols) for biofuels with respect to production systems analysis under the headlines (1) feedstock potential, (2) conversion process to biofuels, (3) economic sustainability assessments (including fuel costs), environmental sustainability assessments (including greenhouse gas emissions), societal sustainability assessments, and (4) distribution infrastructure.

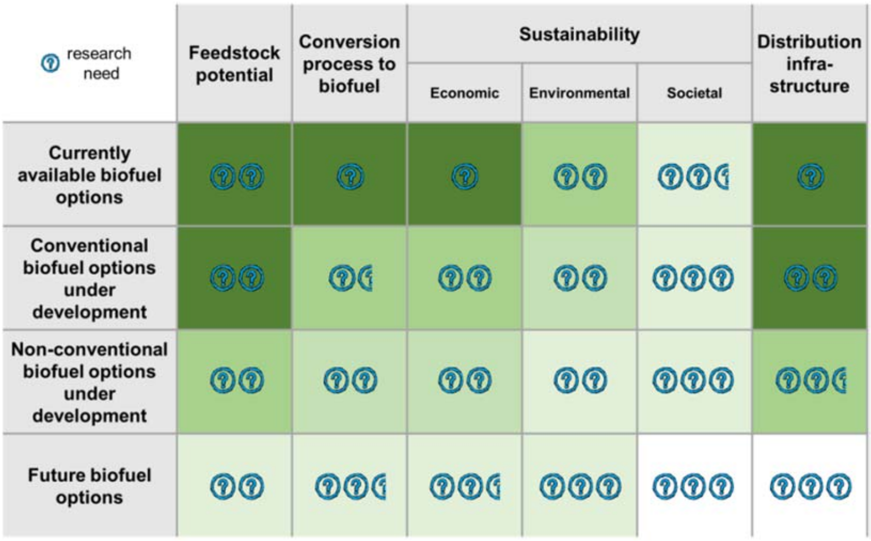

Figure 10: Qualitative assessment of the state of knowledge (shading) and the research need (question mark symbols) for biofuels with respect to production systems analysis. The darker the green, the higher the knowledge level.

In Figure 10 it can for example be seen that a lot of research has been conducted to date around the feedstock potential for current biofuels. However, there still resides considerable uncertainty in the estimates and research efforts are needed to address and reduce this uncertainty. Even for emerging biofuels the feedstock situation is quite well investigated while for future biofuels – e.g. based on algae – the feedstock potential is less well defined. For all biofuel categories however, a certain level of research is still needed to improve estimates of the biomass potential.

Example of more specific topics identified as needing more research:

- Multi-objective optimization of fuel alternatives accounting for parameter uncertainties in order to identify robust fuel pathways for the future.
- Studies accounting for regional differences and opportunities/risks for both feedstock growth and harvest as well as production processes (e.g. integration to existing industry infrastructure).
- Interactions between biofuel production processes and the stationary energy sector, in particular electrofuels are of interest in this regard.

- Better understanding of land use change effects and feedback loops to facilitate decision making in order to avoid biofuel production options with negative effects with respect to greenhouse gas emissions and environmental performance from a systems perspective.
- Social factors – even though not being quantifiable at the same level as economic and environmental ones – need to be included for both fossil and renewable fuels as an additional measure for decision making.

Interdisciplinary research

The overall challenge is to get investments into alternative fuel production. Today it is generally hard to make alternative fuels economically competitive without subsidies. The insecurity regarding which fuel has a future and which are facing major challenges need to be better understood. The vehicle manufacturers have to be involved in the process as well as the fuel producers. This implies that there is a need for interdisciplinary and iterative system and engine research that can quantify the production potential, well-to-tank carbon emissions as well as total cost calculations. The computations have to be made transparent in order for the industry to be involved and accept the results.

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