Well-to-tank data for advanced tailor-made biofuel alternatives

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Purpose and approach

The transport sector accounts for almost 25 % of Europe's GHG emissions and is the main cause of air pollution in cities. As part of the effort to increase the sustainability of the transport sector, and to reach the national vision for a vehicle fleet that is independent of fossil fuels by 2030 Sweden set of goals for an increased share of renewables in the transport sector, also following the EU target of at least 10% by 2020. Within a research collaboration between the Swedish Internal Combustion Engine Consortium (SICEC), Chalmers University of Technology, a large industrial network, and the Swedish Knowledge Centre for Renewable Transportation Fuels f3, advanced tailor-made biofuel alternatives with superior performance to today’s fossil and renewable fuel alternatives are investigated. A key aspect of the research collaboration is a close dialogue between the experimental engine research teams investigating engine performance and biofuel handling and combustion in the engine systems, and the energy systems research groups analyzing the biomass potential, production aspects for the respective biofuels, and performance of the entire value chain from well-to-wheel (WTW). In regular meetings, the results and findings of the research groups are presented and discussed and input from the industrial partners, representing engine manufacturers, fuel suppliers and processing industry is collected and integrated into the further project planning. Based on a pre-study performed prior to the project (Grahn & Sprei, 2015), a set of initial fuels, so-called A-fuels, have been defined for evaluation at the beginning of the project. Based on the results and findings that will be obtained from both engine experiments and systems studies, biofuels - or blends of biofuels - with good WTW performance that can be used in improved combustion engine concepts will be identified. After a first evaluation, it is envisaged to go further with a set of fuels that have been identified having better sustainable production pathways, so-called B-fuels, during the course of work with the A-fuels, that might have similar of even better combustion performance or allow for more advanced combustion engine concepts, and thereby further improving the WTW performance. The project is inspired by – and planning to establish a collaboration with – a German initiative on tailor-made biofuels at RWTH Aachen (TMFB, 2016). Comparison is also made to results on renewable diesel fuel alternatives in the JEC WTW study (JEC, 2014).

The present paper presents preliminary results for the production pathways for the A-fuels chosen for the compression-ignition (Diesel) engine combustion experiments. These eight biofuels are:

- n-octanol
- 2-ethyl-hexanol
- n-decanol
- 2-propyl-heptanol
- DNBE
- 2-MTHF
- Caromax 28
- PolyDME (or POMDME)

An overview of potential production pathways for the eight biofuel alternatives is given and a more detailed analysis for one of the biofuels, 2-ethylhexanol, focusing on WTT energy performance is presented.

Scientific innovation and relevance

The project's major innovation is the cross-disciplinary approach of combing the research disciplines on energy systems research with combustion engine research, adopting a broader perspective. The industry perspective is integrated into the project by the regular working group meetings. The major goal is to contribute with applicable data for promoting the best biofuel alternatives for a medium term future with both improved engine combustion concepts and sustainable production pathways. Feedstock potential and integration opportunities with existing industry infrastructure for improved techno-economic and environmental production performance will also be an inherent part of the biofuels analysis of WTT performance. The project will contribute with additional WTW performance data, striving for comparability to existing studies and a better dissemination of the results.

Results and conclusions

An overview of the potential production pathways for the different biofuels as illustrated in Figure 1 has been established.

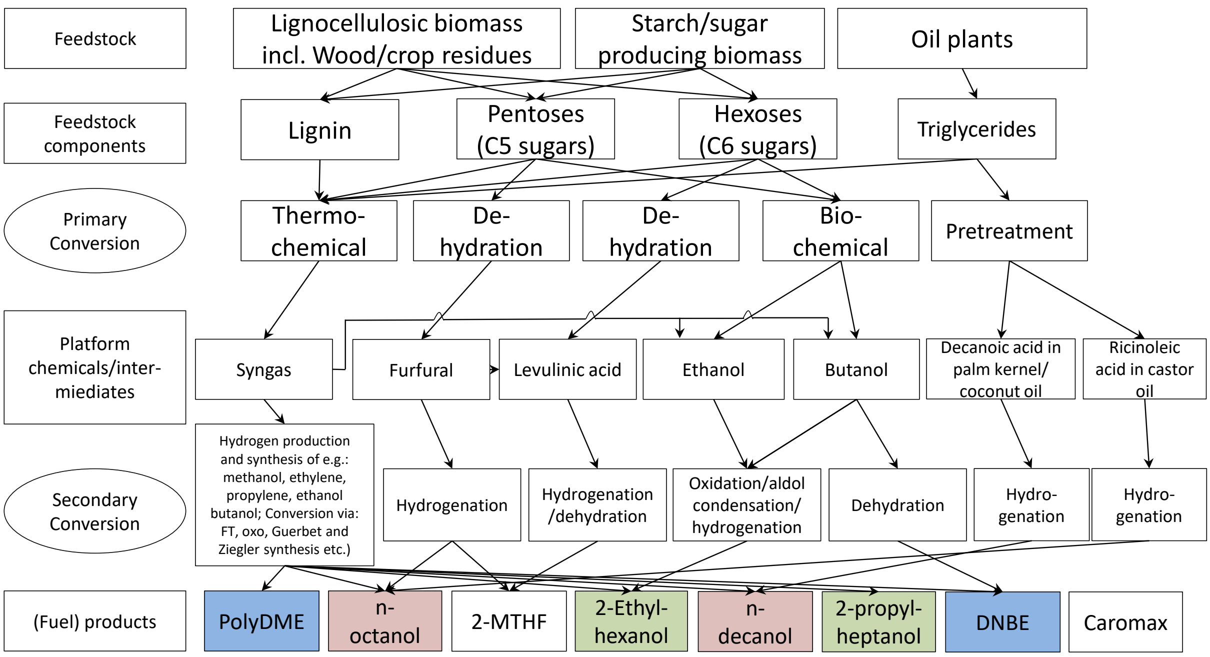

Figure 1: Overview of production pathways for the eight fuels chosen for CI engine experiments (Hackl. 2016).

It can be stated that the vast majority of industrially relevant production pathways for the chosen biofuel alternatives proceeds via platform chemicals or chemical intermediates. Some of these intermediates – such as ethanol or butanol – can directly be applied as biofuels in combustion engines. An important contribution of the overall research project will be to evaluate whether the losses in further refining these intermediates to more advanced biofuels can be justified by superior combustion properties. A multi-criteria analysis of the well-to-tank performance of different pathways will investigate the advanced biofuel performance with respect to environmental, techno-economic and social sustainability. The mass and energy balances for the different pathways constitute a crucial input data to such an analysis. Different pathways will be evaluated and options for process integration leading to potential energy benefits and valorization of co-generated services and products (e.g. electricity or district heating) investigated.

To illustrate the methodology, one of the Diesel-like biofuels – 2-ethylhexanol – has been chosen and three different production pathways are analyzed for their energy performance as a basis for the well-to-tank analysis. 2-ethylhexanol can be produced via the following three routes:

1) *Butanol-based via Guerbet condensation (Gabriëls et al. (2015))*
   Guerbet reaction of two n-butanol molecules leading to the formation of one molecule of water and 2-ethylhexanol.

2) *Ethanol-based via the intermediate product n-butyraldehyde (Eliasson (2010), Raff (2000), Billig (2000))*
   Ethanol is partially oxidized to acetaldehyde in a silver-catalysed process. The acetaldehyde is thereafter converted to crotonalaldehyde which is then hydrogenated to the intermediate chemical n-butyraldehyde. This can then be used to synthesize 2-ethylhexanol.

3) *Gasification-based via OXO-synthesis (Raff (2000) Billig (2000))*
   Syngas and propylene are converted to n-butyraldehyde which is subsequently converted into 2-ethylhexanol and other products.

The performance of the three routes is compared to results for other biofuels serving as Diesel drop-in or substitute from the WTT analysis of the JEC study (JEC, 2014). Combining the present work with life cycle impact assessment and engine combustion experiments will allow to evaluate whether the increased effort for production of advanced biofuels – that often are based on intermediates such as ethanol or butanol that could be directly used as fuels – can be motivated by the improved combustion engine performance, thus leading to superior WTW performance. Critical aspects with respect to biomass potential and integration opportunities with existing industry infrastructure will be highlighted for the different fuels in future work as well.

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