Evaluation and further development of a spreadsheet-based calculator to estimate the properties of naphtha-type biofuels

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Abstract
The ability to predict the combustion properties of novel second-generation biofuels is key in the process of defining their usability as fuels for internal combustion engines. Within the framework of the Belgian Government funded Ad-Libio project, investigation of the potential of light-naphtha biofuel is being performed by means of developing a freely available fuel component database and a fuel blend calculator. The database and the calculator are being modified from previous work conducted at the RWTH Aachen University and the University of Bath. The focus will be to develop the calculator in such a way that it can accurately predict the properties of the naphtha-type biofuels and blends within the Ad-Libio project. However, the calculator may be useful for the development of other sustainable fuel alternatives, making it a versatile tool in novel fuel development.

Key words
Blend calculation, Fuel database, naphtha-type fuels, biofuels

Introduction

A future sustainable transport system is dependent on finding new ways of producing second-generation (2G) biofuels that are not in competition with food agriculture. A novel biofuel production process using woody biomass without the need of enzymatic saccharification was developed by researchers at KU Leuven [1]. In short, 2G biomass is mechanically milled, lignin is catalytically extracted in a first step and the remaining (hemi)cellulose is catalytically converted into light C5-C6 naphtha streams, see Figure 1. The use of catalytic conversion makes the process less CO_2 intensive than its enzymatic counterpart. Furthermore the reactions occur at relatively low temperatures and pressures, compared to gasification, pyrolysis or liquefaction. This process produces naphtha-type biofuels referred to as Advanced Liquid Biofuels (Ad-Libio). The Belgian federal government has funded a project aiming to further develop this process, but also to evaluate the potential of the fuel in different combustion concepts.

The Ad-Libio fuels contain a mixture of straight-chain hydrocarbons (83 vol%), branched or cyclic hydrocarbons (16 vol%), and oxygenated compounds (1% furans) with a chain length of 5 to 6 carbon atoms [1]. However, the composition could be varied slightly to impact the combustion properties. For naphtha-like fuels, compliance with current fuel standards (EN228 and EN590) may be achieved by blending them with fossil fuels or other biofuels.

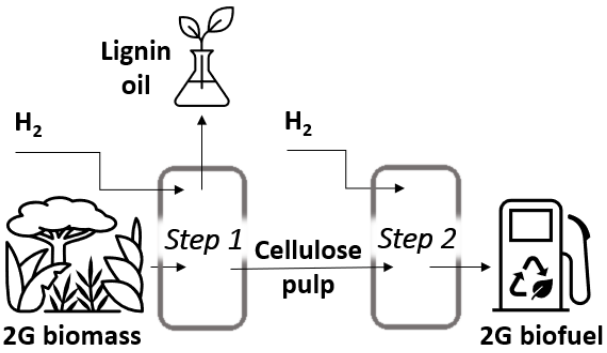

Figure 1. Conceptual overview of the Ad-Libio production process.

In order to investigate the usability of fuel blends containing Ad-Libio fuel components, an Excel-based fuel blend property calculator [2] was tested in combination with an extensive fuel property database from vom Lehn et al. (RWTH Aachen University) [3]. While performing the property

calculations it was found that there are some limitations to the calculator and the database alike, making it difficult to get a full picture of the potential of the Ad-Libio fuel blends [4]. Therefore, efforts have been made to further develop the fuel calculator and the database to accommodate the evaluation of the fuel mixtures of interest for the Ad-Libio project and for the evaluation of other future biofuel mixtures.

Research Methodology

The fuel blend calculator expands the current fuel database with properties related to compression ignition and fuel spray characteristics, since the database originally emphasizes spark-ignition engine applications [3]. To be able to evaluate novel fuels where experimental values are limited, methods using the chemical structure of the fuel component (QSPR-methods) [5] will be preserved from the fuel database from Aachen, but are being adapted to include the extended properties. Furthermore, experimental values of fuels that consist of multiple components (gasoline, diesel, RME etc.) are being added to the fuel database.

The fuel blend calculator is being developed to become an extension of the calculator developed by Vinke at the University of Bath [2] with added properties related to diesel fuel standards. Activity coefficients or empirical equations from literature are being added for the properties where the addition of oxygenated compounds (mainly alcohols) has exhibited non-linear behaviour when mixed with hydrocarbon fuels [6]. The number of inputs is increased, as well as the input resolution, to allow for higher precision in the volumetric ratio of the components.

All calculations will be evaluated against data from previous published references, and in the future against data obtained within the Ad-Libio project.

Future objectives

The fuel calculator is a work in progress and needs to be further developed with previously mentioned additions in mind. Future work will include evaluation of the calculator against references and measured values, development of a user friendly and intuitive interface, and the addition of more fuels and measured fuel properties.

In parallel with the development of the calculator itself, the compliance of the Ad-Libio fuels and blends with current fuel standards are being evaluated. The potential of these fuels with different combustion concepts will also be investigated, with the first emphasis being on the potential of Ad-Libio fuel blends for spark-ignition engines.

Summary

Within the Ad-Libio framework, efforts are being made to improve a publicly available spreadsheet-based fuel database and a fuel property calculator. The calculator will be able to perform preliminary calculations estimating several combustion-related properties of fuel blends. At the current stage the development of the calculator will be verified for the naphtha-type fuels within the Ad-Libio project.

The fuel database and property calculator combination offers great potential for the creation of a versatile tool that can be used for future evaluation of other novel fuel alternatives.

References

1. de Beeck, B.O., et al., *Direct catalytic conversion of cellulose to liquid straight-chain alkanes.* Energy & Environmental Science, 2015. **8**(1): p. 230-240.
2. Vinke, I., *Development of a fuel mixture properties calculator with preparation for web-based implementation.* 2020.
3. vom Lehn, F., et al., *A property database of fuel compounds with emphasis on spark-ignition engine applications.* Applications in Energy and Combustion Science, 2021. **5**: p. 100018.
4. Tom Robeyn, S.V., Immanuel Vike, Hannes Latine, Jamie Turner, *Investigation of naphtha-type biofuel from a novel refinery process.* 2022.
5. Shi, C. and T.B. Borchardt, *JRgui: A Python program of Joback and Reid method.* ACS omega, 2017. **2**(12): p. 8682-8688.
6. Christensen, E., et al., *Renewable oxygenate blending effects on gasoline properties.* Energy & Fuels, 2011. **25**(10): p. 4723-4733.