“Investigating the potential of advanced tailor-made biofuels – A well-to-tank environmental analysis of 2-ethylhexanol as a drop-in diesel alternative”

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The present study evaluates the environmental performance of 2-ethylhexanol (2-EH), as a potential drop-in biofuel alternative. Three different bioenergy production pathways are investigated; ethanol-based, gasification-based and butanol based. Considering the overall energy efficiency, the different pathways show similar performance, with the gasification route exhibiting slightly higher values. When only 2-EH production is concerned, the butanol based route results in the lower primary energy demands. In comparison to other biofuels 2-EH can provide a competitive alternative since fossil fuel dependency is decreased without considerable infrastructure changes.

Introduction

Advanced tailor-made (TM) transport fuels based on renewable feedstock are promoted as alternatives towards increasing the share of biofuels in today’s vehicle fleet. As part of a national Swedish research project such fuels are investigated with the aim to identify and suggest drop-in alternatives that offer not only excellent combustion properties but also assist in improving the sustainability performance of the transport sector along its value chain. Technical, economic and environmental performance criteria are integrated in the assessment process of the different fuels. The present work focuses primarily on the environmental performance of the different alternatives assessed in the project. Through a case study on 2-ethylhexanol (2-EH), preliminary results are provided.

2-EH is an eight-carbon alcohol used as platform chemical to produce plasticizers, coatings and other speciality chemicals [1]. New research shows that 2-EH could also provide a promising drop-in alternative for transport fuels [2]. Conventionally, 2-EH is produced from the conversion of fossil propylene and syngas (a mix of H_2 and CO) to n-butyraldehyde followed by a condensation and hydrogenation reaction to yield 2-EH. Although not commercially available yet, the production of 2-EH from renewable feedstock is also possible [3].

Approach

The environmental impact of 2-EH is estimated using attributional life cycle assessment (LCA) [4]. The assessment includes the activities of biomass acquisition and conversion, production of intermediate chemicals and synthesis of the final fuel (2-EH). Transports of raw materials to the main facility are also considered. All conversions from feedstock to fuel are assumed to take place at the same facility which eliminates the need for transports and benefits from heat exchanges and energy recovery. Fuel distribution is excluded as it considered an identical activity for all processes.

The functional unit is defined as 1 MJ of renewable 2-EH with a lower heating value (LHV) of 37.6 MJ/kg. To produce 2-EH, three different bioenergy pathways are compared; ethanol-based, gasification-based and butanol based (Fig 1).

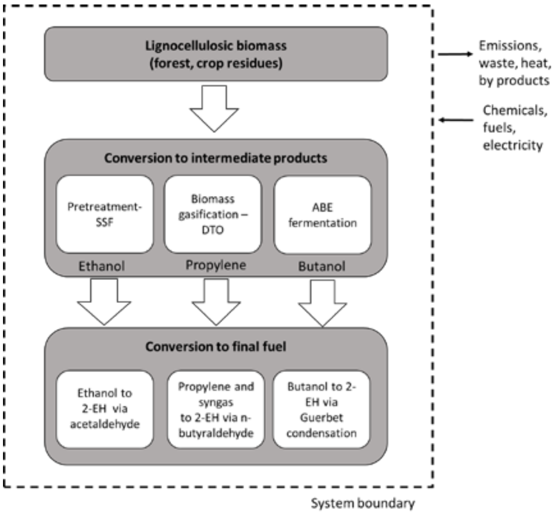

Fig. 1: Production pathways for 2-ethylhexanol (2-EH) assessed in this work

Data for the different processes were collected through scientific articles and industry reports. Background activities (e.g. raw materials production, electricity production, transports etc.) were modelled using the Ecoinvent v2.2 life cycle inventory database [5].

As biorefineries produce more than one product, allocation issues emerge [6]. System expansion with product substitution was assumed to model multioutput processes and to determine the environmental burden of the desired product.

The two impact categories presented here are Cumulative Energy Demand (CED) expressed in MJ and Global Warming Potential (GWP) expressed in kg of carbon dioxide (CO_2) equivalents, following the methodologies described in [7]. The study was modelled using OpenLCA v1.6 [8].

Process description and assumptions

A short description of the three different production processes for 2-EH is provided below. A selection of inventory data is listed in Table 1. Chemicals and

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other inputs are not shown in the table due to confidentiality issues in relation to some of the pathways.

Table 1: Selection of inventory data for 2-EH production under the three different pathways

	2-EH via ethanol	2-EH via gasification	2-EH via butanol
Input (in MW)			
Forest Biomass (50%mc)	244.0	100.0	
Corn stover (20%mc)			373.0
Electricity	16.8		
Hydrogen	25.0	2.7	
Steam/Heat	36.0*		
Output (in MW)			
2-EH	**82.9**	**21.4**	**122.0**
Biogas	3.4		
Lignin	97.6		
Ethylene		18.9	
C4 compounds		8.8	
Electricity			11.1
Acetone			5.6
Ethanol			18.6

*heat demand is covered from the biogas produced in the process

2-EH via ethanol

Forest biomass is converted to ethanol through a simultaneous saccharification and fermentation (SSF) process based on the SEKAB technology developed in Sweden. Data on inputs and yields were obtained from the Swedish Forest Chemistry project [9] where lignin, biogas and carbon dioxide (CO_2) are delivered as by-products. The obtained biogas is used internally to cover the heat and steam demand of the process. Lignin could also be used to provide electricity for the process, although import of additional electricity would still be needed. For this reason, product substitution was investigated instead in two scenarios. In the first scenario, the electricity produced from lignin (assuming 35% conversion efficiency) is all exported to substitute marginal electricity from coal. Moreover, lignin is considered a promising replacement to different fossil based feedstocks and materials including carbon fibers thus a second scenario, considers the substitution of polyacrylonitrile (PAN), the precursor of carbon fibers based on data provided by Das [10].

The conversion of ethanol to 2-EH is done in two steps where ethanol is first converted to acetaldehyde [11] and then acetaldehyde is converted to 2-EH. The energy demand and conversion efficiencies for the latter conversion are estimated starting from an acetaldehyde to n-butanol process [12] with similar layout. The hydrogen necessary for this process is produced by electrolysis (assuming 65% efficiency from electricity to hydrogen [13]).

2-EH via gasification

This pathway, follows the traditional 2-EH production route with the difference that forest biomass is used instead of fossil feedstock. Syngas (from biomass gasification) is converted to DME followed by a DME to olefins (DTO) process to obtain propylene. Data for these conversions were obtained from Arvidsson et al. [14]. Besides propylene, the DTO process results in ethylene and other C4 compounds. Fossil propylene and butene (assumed for C4 compounds) were considered as avoided products. Their impact was modelled based on the processes described in Ecoinvent v.2.2.

The conversion from propylene to 2-EH (OXO-synthesis) involves several conversion steps and byproducts and yields both n- and i-butyraldehyde as well as some butanol, off-gases and heavy ends. All C4 fractions are assumed to be further converted to 2-EH or to n- and i-butanol. The conversions and yields for the OXO-synthesis for 2-EH production from propylene are based on [15, 16].

2-EH via butanol

This pathway, follows the Guerbet reaction where 2-EH is obtained from n-butanol at very high rates (nearly 99%). N-butanol is obtained through the acetone-butanol-ethanol (ABE) fermentation process as described in Tao et al. [17]. Corn stover was assumed as biogenic feedstock. Corn stover production was modelled according to Murphy and Kendall [18].

During the ABE process acetone, ethanol and solid residues (including lignin) are also produced. The solids are burned to cover all energy demands for the ABE and subsequent 2-EH production process. Excess electricity was assumed to be exported to replace marginal electricity from coal while fossil acetone and gasoline were assumed as avoided products.

Results

Considering the overall energy efficiency (total input and total output energy), the three pathways can be ranked in the following order: gasification pathway (55%) > ethanol pathway (47%) > butanol pathway (46%). When only 2-EH is concerned this figure slightly differs with the butanol pathway becoming the more energy efficient alternative (33%) followed by the ethanol (22%) and the gasification pathway (21%). This is indicated also by Figure 2 where the CED indicator to produce 1 MJ of 2-EH is illustrated. CED represents the total primary energy demand of the three pathways including both renewable and fossil resources. The bars in the figure show the energy input (positive values), the potential savings (negative values) when substitution alternatives are concerned, as well as the net energy requirements (black points).

2-EH via butanol, results in lower net CED. The gasification pathway results in high CED, although the majority is due to the biomass input (i.e. renewable energy). When fossil energy is concerned, activities that result in high primary energy needs are enzyme and chemicals production especially for the ethanol and butanol based pathways.

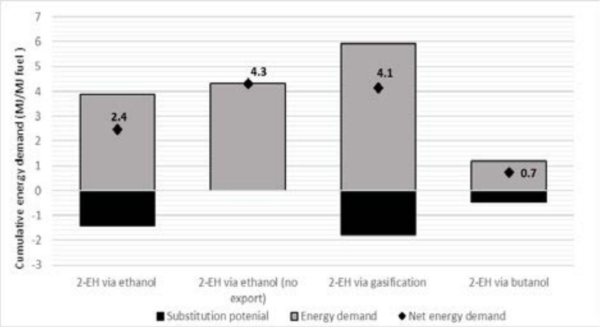

Fig. 2: Environmental assessment of 2-ethylhexanol under different production pathways. Results illustrating the CED indicator.

In terms of GWP, the butanol route exhibits highest net greenhouse gas (GHG) emissions while for the gasification and ethanol routes the net GHG emissions per MJ 2-EH are almost zero (due to the fossil product alternatives replaced). GHG emissions for all pathways result mainly from background activities. In line with previous research, enzyme production is responsible for a significant share.

The results can be sensitive to the assumptions in relation to the substitution alternative or allocation method. For the ethanol pathway, under the assumption that lignin will be used internally (as in the butanol case) the net energy demand increases while when PAN fibers are replaced the net CED and GWP indicators are reduced substantially and even result in negative values.

Discussion and conclusions

A preliminary assessment of 2-EH in terms of energy requirements and GWP is provided. Compared to the intermediate fuels obtained (ethanol, butanol) or other biofuel alternatives as the ones presented in the detailed analysis by Edwards et al. [13] the energy inputs for 2-EH can be higher due to the additional conversion steps required.

From a systems perspective, several parameters are expected to influence the fuel mix of the future transport sector. Such parameters include the share of renewable feedstock in the fuel, combustion behavior, infrastructure needs, production potential and cost. With 2-EH, highly renewable blends can be achieved limiting the need for fossil feedstocks. Experimental results showed that the use phase performance of 2-EH was comparable to diesel with lower emissions of soot or hydrocarbons [2]. Compared to ethanol or DME, the need for infrastructure changes or engine modifications are also lower. Production cost can be higher however, due to the additional steps. Further investigations in relation to the use phase performance as well as other environmental and cost performance indicators are needed to provide a comprehensive analysis of such novel fuels.

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