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RESEARCH ARTICLE

Lifecycle energy and greenhouse gas emissions analysis of biomass-based 2-ethylhexanol as an alternative transportation fuel

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Abstract

This study investigates the environmental performance of 2-ethylhexanol (2-EH), as a potential drop-in transport fuel alternative. Three different biomass-based production pathways are evaluated and compared using life cycle assessment (LCA) methodology. The environmental impact of 2-EH is assessed in terms of cumulative energy demand (CED) and global warming potential (GWP). Among the three alternative pathways, 2-EH produced via syngas results in the lowest primary energy demand and GHG emissions under the baseline assumptions of this work. The two biochemical production pathways (via ethanol and butanol) exhibit higher CED and GWP during biomass conversion steps mainly due to process materials and chemicals used. Process specifications such as transport distance to production facility or the fate of the obtained by-products are shown to influence the overall environmental impact of the fuel for all studied pathways. The use phase performance of 2-EH was also considered in this work, as part of a 100% renewable blend and was compared to existing fossil and renewable fuels. The studied blend has the potential to reduce GHG emissions by more than 85% compared to fossil diesel while when certain production pathways are followed, it exhibits lower GWP than renewable fuels already in the market such as ethanol blends and biodiesel. 2-EH can therefore provide a competitive alternative to fossil transport fuels increasing the share of renewable content in the current vehicle fleet, thus enhancing the efforts for a sustainable transport sector.

KEYWORDS

2-ethylhexanol, climate change, drop-in fuels, life cycle assessment, renewable fuels, transportation

1 | INTRODUCTION

Under the recent Paris Agreement, more than 180 countries agreed to mitigate climate change and suggested ambitious targets for reducing their greenhouse gas (GHG) emissions.¹ The implications for the transport sector are substantial. The European Union (EU) strives for a 60% reduction in GHG emissions from transports compared to the 1990 levels, by 2050.² The former target of 10% of renewable fuels in the

vehicle fleet by 2020³ is changed to a minimum share of 14% by 2030 in the revised renewable energy directive (RED) that is expected to enter in force by the end of 2018.⁴

For the time being, the vehicle fleet is dominated by fossil-based fuels which is one of the main obstacles in realizing these goals, as emissions from road transport tend to increase.⁵ About 95% of the European fleet consists of diesel- or gasoline-driven vehicles. Low-carbon renewable fuels and alternative powertrains (such as electric vehicles) account for

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only a minor share. These, in combination with rising transport demand, pose a challenge to the sustainability of the sector and require actions both from a long- but also short-term perspective.

In the long term, a fossil free and energy efficient transport sector is envisioned. To enhance this transition and at the same time to continue reducing the impact of transports, actions in the short-term are essential. While electrification of the transport fleet may require further technological as well as infrastructure development, before it becomes a widely applied alternative, using the current fleet in a more effective way and enriching it with advanced, renewable and low emission fuels could be among the short- to medium-term solutions.

Biomass-based liquid fuels have been available for many years. Resource constraints and the risk for competition with food production along with other aspects such as production cost, fuel handling and distribution, and the needs for engine modifications have slowed down the expansion of certain types of renewable fuels.⁶ Second generation, or advanced biofuels, produced from waste and crops or forest residues, handles some of these limitations providing a more sustainable and viable option.^{3,7}

Interest for “drop-in” and “tailor-made” renewable fuels has increased significantly in recent years. Drop-in fuels can be blended with conventional fuels at high concentrations. As such, drop-in fuels require few to no modifications of existing vehicle powertrain technology and can be handled, stored, and transported through the existing fuel infrastructure.⁸ Research on fuel design has further facilitated the development of tailor-made fuels that is customized fuels that aim to combine improved combustion performance and sustainable fuel production processes.⁹ Long-chain alcohols and fuels with high-oxygen content are considered promising candidates providing alternatives both for spark ignition (SI) and compression ignition (CI) engines.^{9–11} Alcohols such as n-octanol or n-decanol (C_8 – C_{10}) have densities similar to diesel while their increased-oxygen content assists in decreasing soot and other tailpipe emissions.¹²

Experimental work around these novel fuels illustrates their benefits in terms of engine performance.^{12–15} These fuels can be produced from lignocellulosic biomass increasing the interest in their development. To provide a comprehensive picture and to minimize the risk for suboptimizations along their value chain, holistic investigations are needed. This type of investigations should combine production pathways analysis with life cycle environmental performance assessments in order to complement the fuel's use phase performance assessments.

A branched long chain alcohol and isomer to octanol—2-ethylhexanol (2-EH)—is selected to be studied in this work. Biomass-based production of 2-EH has been subject to investigations earlier by Patel et al¹⁶ who also assessed the life cycle performance of 2-EH production from ethanol. 2-EH

is used mostly as a platform chemical to produce plasticizers, coatings and other specialty chemicals. The large-scale fossil-based production of 2-EH is based on the conversion of propylene and syngas to n-butyraldehyde and a condensation and hydrogenation reaction to yield 2-EH via 2-Ethylhexenal. Propylene is most often produced by steam cracking of fossil oil, whereas the syngas is generally produced through steam reforming of natural gas.¹⁷ As shown in Hackl,¹⁰ 2-EH can also be produced from biomass-based material. The use of 2-EH in the automotive sector is not new, although using 2-EH as a transport fuel brings out a new application and business area. 2-EH can be blended with conventional diesel or renewable fuels such as hydrogenated vegetable oil (HVO) or rapeseed-methyl-ester (RME) offering the possibility to achieve a fuel with highly renewable energy content. Engine performance characteristics of 2-EH blends have been investigated by Preuß et al¹² and Zhang et al¹⁵ showing promising results in terms of thermal efficiency as well as reduced regulated emissions.

As fuel combustion characteristics have been already assessed, the primary aim of this work was to further investigate the environmental performance of biomass-based 2-EH from a life cycle perspective with a focus on primary energy demands and GHG emissions.

Three different biomass-based production pathways are presented and evaluated including all activities from biomass extraction to fuel production. The three production pathways considered are denoted as:

- Pathway A: 2-EH_{Ethanol}, where 2-EH is produced through biomass fermentation with ethanol as intermediate chemical.
- Pathway B: 2-EH_{Syngas}, where 2-EH is produced through biomass gasification with syngas and propylene as intermediate chemicals.
- Pathway C: 2-EH_{Butanol}, where 2-EH is produced through acetone–butanol–ethanol (ABE) fermentation of biomass with butanol as intermediate chemical.

An additional aim of this paper was to compare and benchmark the use phase performance of 2-EH in a 100% renewable blend against conventional fossil and biomass-based alternatives and therefore providing the opportunity for a holistic well-to-wheel (WTW) performance assessment of this fuel. Based on the outcome of this work, the availability and supply potential of 2-EH as transport fuel is also discussed from a resource perspective.

2 | MATERIALS AND METHODS

The environmental performance of 2-EH is assessed using Life Cycle Assessment (LCA), following the international

standard ISO 14044.¹⁸ LCA is a commonly applied tool for investigating the environmental performance of products or services throughout their life cycle; from resource extraction, to production, use and final disposal.¹⁹ In addition, and to facilitate comparisons to other studies on transport fuels, the methodology provided by the European renewable energy directive (RED) is used.³ Differences between the two approaches are described below when relevant.

2.1 | Goal and scope of the study

The present work follows the attributional LCA modeling approach. The purpose of the study was to assess the environmental performance of 2-EH, as a potential drop-in transport fuel alternative. This is done by analyzing and comparing different biomass-based production pathways based on current available data. To investigate the potential of this novel fuel, an explorative future-oriented scenario is investigated as sensitivity analysis.

The three pathways and life cycle stages considered in this analysis are illustrated in the generic flowchart provided in Figure 1. In Section 2.3 the system's specifications are described, and details on the most significant methodological assumptions are provided.

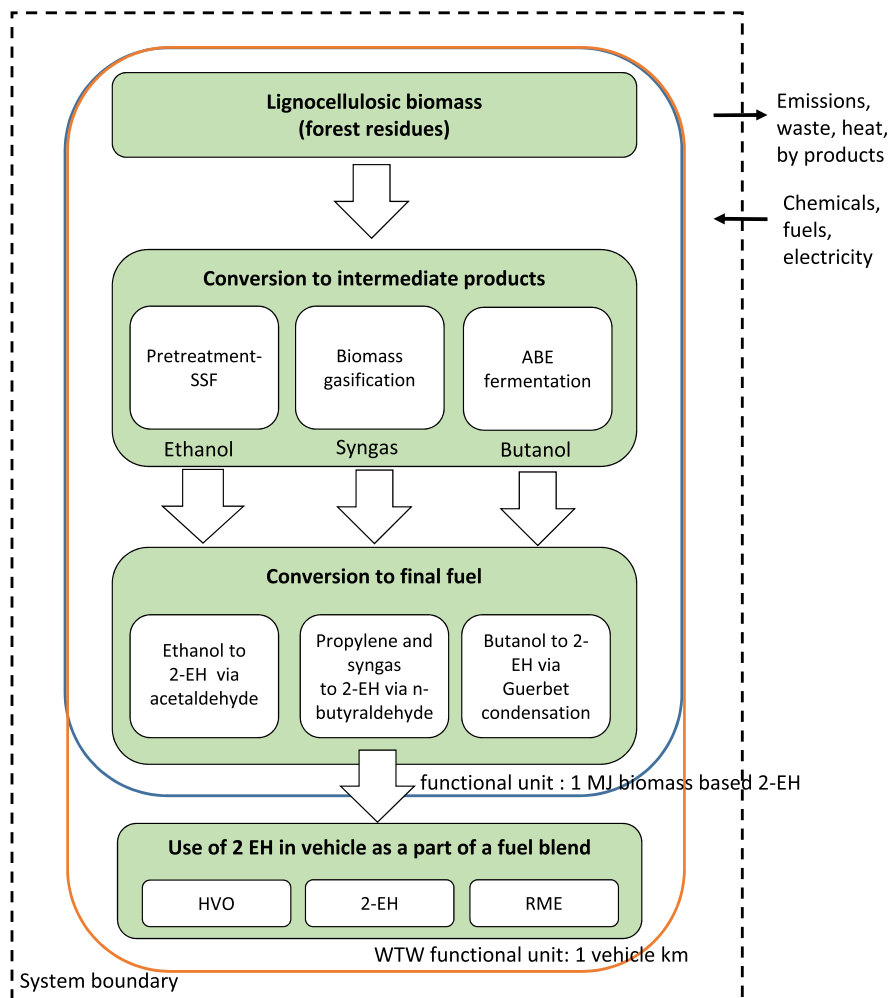
The assessment covers the activities of biomass acquisition and conversion, production of intermediate chemicals and synthesis of the final fuel (2-EH). Transports of raw materials to the main facility are also included. Distribution of 2-EH to fueling stations is excluded as it is considered to be identical for all pathways. The functional unit is defined as 1 MJ of biomass-based 2-EH, with a lower heating value (LHV) of 37.6 MJ/kg.

For the WTW comparison to existing fuels, a 100% renewable fuel blend for diesel engines is considered, consisting of 2-EH, HVO (from tall oil) and RME according to data provided by Preuß et al¹² A blend (instead of neat 2-EH) is selected in order to fulfill the existing fuel standard and provide a fuel with similar quality and properties to diesel. The functional unit is revised to 1 vehicle km (see Figure 1) and the life cycle stages of both fuel production and use are included for all fuels considered for comparison.

2.1.1 | Multifunctional processes

Chemical conversions and biorefinery systems often produce more products than the product in focus.²⁰ Multi-output processes in this work have been handled by using

FIGURE 1 Generic flowchart showing the life cycle stages and production pathways for biomass-based 2-ethylhexanol (2-EH) considered in the assessment. The system boundaries of the study are shown. The blue border indicates the system boundaries of the environmental assessment of 2-EH where the functional unit is defined as 1 MJ of biomass-based 2-EH. For the well-to-wheel (WTW) analysis and comparison to other fuels (orange border), a fuel blend is considered, and the functional unit is revised to 1 vehicle km. ABE, acetone–butanol–ethanol fermentation; HVO, hydrogenated vegetable oil; RME, rapeseed-methyl-ester; and SSF, simultaneous saccharification and fermentation process



the system expansion approach as recommended by LCA guidelines.^{18,21} Product substitution (a form of system expansion) was applied in all baseline cases following the ISO methodology. Substitution in practice means to subtract the inventory of another system from the analyzed system, thus a negative inventory flow is created.²¹ By-products are assumed to substitute existing equivalent products, thus the burden from producing these can be subtracted from the studied system.

In RED, an alternative way to deal with multi-functionality is applied based on allocation or partitioning of the environmental burden across the different outputs of the process using physical criteria and more specifically the energy content of the different products.³ The way that multifunctional processes are handled influences the outcome of the study, thus differences in the outcome between the ISO and RED approaches can be expected.^{20,22}

2.2 | Data sources and modeling

Data for the different processes were collected through scientific articles, industry reports, personal communication with relevant actors as well as the authors' own calculations. For background activities (i.e. production of raw materials, electricity and fuels)

data from the Ecoinvent v3.3 life cycle inventory database were used.²³ The LCA model was built in OpenLCA v1.7²⁴ including the inventory model and impact assessment.

2.3 | Production pathways of 2-EH. System description and inventory data

The mass and energy balances for the three production pathways are summarized in Table 1. The consecutive sections provide an overview of the conversion processes and assumptions of the study. Further details can be found in Heyne et al.²⁵ All energy flows are expressed on a lower heating value (LHV) basis. The efficiency metrics presented in the table are the biomass to fuel efficiency η_{bio} and the overall efficiency η_{tot} , as defined in equations 1 and 2, respectively:

$$\eta_{\text{bio}} = \frac{\dot{m}_{2\text{-EH}} \cdot \text{LHV}_{2\text{-EH}}}{\dot{m}_{\text{bio}} \cdot \text{LHV}_{\text{bio}}} \quad (1)$$

$$\eta_{\text{tot}} = \frac{\sum_o \dot{m}_o \cdot \text{LHV}_o + \dot{Q}^- + P_{\text{el}}^-}{\sum_i \dot{m}_i \cdot \text{LHV}_i + \dot{Q}^+ + P_{\text{el}}^+} \quad (2)$$

With \dot{m} being the mass flow, LHV the lower heating value, \dot{Q} heat flow and P_{el} electricity for the respective streams.

		2-EH Production pathways		
		2-EH _{Ethanol}	2-EH _{Syngas}	2-EH _{Butanol}
Input	Biomass (50 wt-% m.c. forest residues)	100 MW	100 MW	100 MW
	Total heat demand	15 MW	44.9 MW	38.4 MW
	Heat import ^a	–	–	–
	Total electricity demand	23 MW	18.6 MW	9.6 MW
	Electricity import	5.2 MW	0.9 MW	–
Main product	2-EH	33.9 MW	27.5 MW	32.7 MW
By-products	Biogas ^a	18 MW	–	18.5 MW
	Biogas export	–	–	–
	Lignin ^a	40 MW	–	37 MW
	Lignin export	–	–	–
	Electricity export	–	–	1.2 MW
	Ethylene (C ₂)	–	18.9 MW	–
	Butylene (C ₄)	–	8.8 MW	–
	i-Butanol	–	1.5 MW	–
	Acetone	–	–	1.5 MW
	Ethanol	–	–	5.0 MW
Efficiency metrics	η_{bio}	33.9%	27.5%	32.7%
	η_{tot}	32.2%	56.2%	40.4%

TABLE 1 Energy balance (LHV basis) during 2-ethylhexanol production under the studied conversion pathways (the figures refer to the baseline scenarios for by-products handling). For underlying assumptions and references refer to sections 2.3.1 to 2.3.3

^aHeat demand of the process is covered internally also generating electricity using CHP; for the ethanol- and butanol-based pathways by-product streams (biogas from waste stream fermentation & lignin) are burnt; covering all heat and electricity demand by imports would allow for exporting these by-products. For the gasification pathway heat for CHP generation is recovered from synthesis gas cooling.

The subscripts and superscripts denote outputs (2-EH, o , and “-”) and inputs (bio, i , and “+”), respectively.

For all pathways, forest biomass (in form of softwood residues) was assumed as feedstock material. The average distance from residues collection to the main facility was 300 km for all pathways using EURO 6 compliant diesel trucks. The transport distance is representative of a potentially relevant location for a 2-EH production site in the vicinity of a chemical cluster at the Swedish west coast. Additional scenarios in relation to distance and fuel were tested using sensitivity analysis. All conversions from feedstock to the final fuel were assumed to take place at the same facility which eliminates the need for transports and benefits from process integration possibilities using the biorefinery concept.²⁶

2.3.1 | Pathway A: 2-EH through biomass fermentation and ethanol

The ethanol-based 2-EH production route is based on a cellulosic ethanol production process, followed by acetaldehyde production and conversion to crotonaldehyde, n-butyraldehyde and finally aldolization and hydrogenation to 2-EH.^{27,28}

Forest biomass is first converted to ethanol through a simultaneous saccharification and fermentation (SSF) process based on the CelluAPP[®] technology developed by SEKAB in Sweden. Process input data were obtained through the Swedish Forest Chemistry project.²⁸ The enzyme cocktail for the process is assumed to be purchased by the Danish company Novozymes A/C and transported from Denmark to Sweden.

Data regarding the environmental performance of the enzyme product were provided by the enzyme supplier after personal communication and were estimated to be 39 MJ of primary energy demand and 0.64 kg carbon dioxide equivalents (CO₂eq) per kg of enzyme product.²⁹ These values are considerably lower compared to data found in previous publications^{7,30,31} due to continuous process improvements as well as geographical variations in enzyme production. The current energy used during enzyme production in Denmark is primarily based on renewable sources. For other nutrients and chemicals needed in the process, inventory data from the Ecoinvent database were utilized.

During ethanol production, solid residues (mainly in the form of lignin), biogas (produced from anaerobic digestion of the liquid effluent streams) and biogenic carbon dioxide are delivered as by-products. Biogas and lignin are assumed to be used as fuels in a combined heat and power (CHP) plant to cover the internal heat and power demand (assuming steam data of 470 °C and 90 bar, boiler efficiency of 0.92 (LHV basis) and turbine isentropic efficiencies of 0.9). The cogenerated electricity reduces the demand for electricity import by

17.7 MW. In this study, carbon dioxide was not considered a by-product, due to market uncertainties.³²

The hydrogen necessary for the process is produced by electrolysis using electricity from the Swedish grid assuming 65% efficiency from electricity to hydrogen.³³ The by-products obtained during 2-EH production (such as heavy ends and gases) are limited and assumed to be used internally to provide heat to the process (Figure 2).

2.3.2 | Pathway B: through biomass gasification and syngas

This production route follows the fossil-based production pathway as illustrated in Figure 3. The process starts with biomass gasification to obtain syngas which in turn is used to produce propylene. Propylene can be produced as a fraction of light olefins via methanol or dimethyl ether (DME) from biomass-gasification.^{34–36} As the syngas for the DME process route is shifted to a H₂:CO ratio of 1, that can be directly used in downstream n-butyraldehyde synthesis, this process route was selected for the purposes of our study. The details for the underlying process assumptions are given in Heyne et al.²⁵

Hydrogen used in the 2-EH synthesis could also be provided from syngas for the given pathway using, for example, membrane separation. For the present study, hydrogen supply by electrolysis is assumed; however, in order to harness the potential synergy effects that can be achieved by supplying part of the oxygen to the gasification, thereby reducing the demand for air separation, a conversion efficiency of 65% (LHV basis) is assumed for the electrolysis.³³

As illustrated in Figure 3, a number of by-products are generated: ethylene and butylene during the dimethyl ether to olefins (DTO) process and i-butanol during the 2-EH synthesis. The ethylene and butylene generated are assumed to replace their fossil counterparts according to the product substitution methodology. In the RED method estimations, propylene is allocated 46% of the upstream emissions and energy demands.

The DTO process is an exothermic process, generating enough heat to cover the additional heat demand of the 2-EH synthesis. As the excess heat is available at high temperature, the integration of a steam cycle for cogeneration of electricity is considered, as in the work of Arvidsson et al.³⁴ The cogenerated electricity (17.5 MW) can cover a large share of the overall process electricity demand (18.6 MW).

2.3.3 | Pathway C: through ABE fermentation and butanol

The 2-EH production pathway through Guerbet condensation of n-butanol (Figure 4) is based on published data for corn stover-based acetone-butanol-ethanol (ABE) fermentation.³⁷ However, this process has been adjusted to account for forest

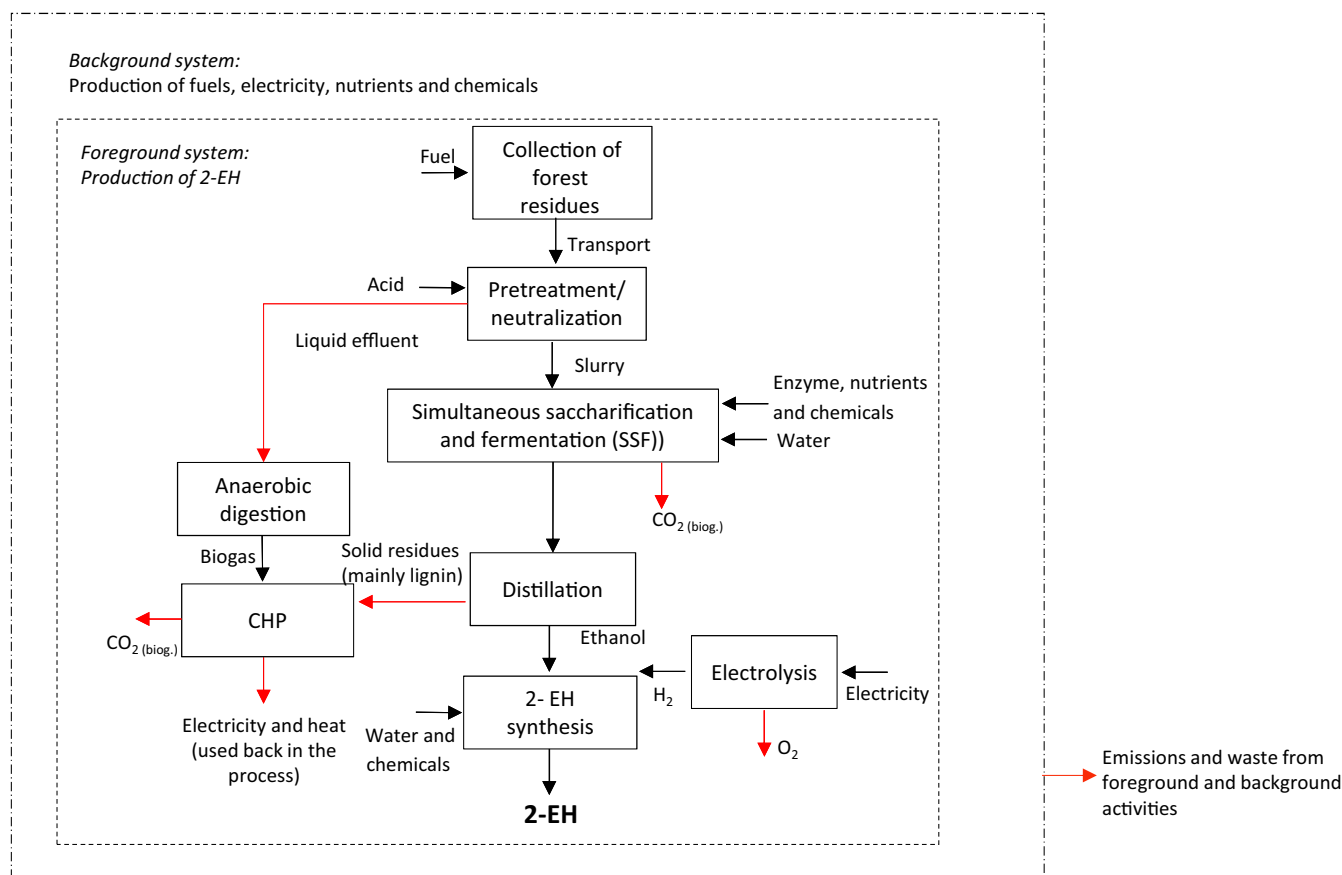


FIGURE 2 2-ethylhexanol production pathway through biomass fermentation and ethanol as intermediate chemical

residues as feedstock using published data for both corn stover and forest ethanol.^{38,39} The specific electricity demand for the ABE process is based on underlying data for the corn stover ABE fermentation.³⁹ To account for the increase in electricity demand for solids handling when switching from corn stover to forest residue, the original data have been recalculated to values specific to dry feedstock flow. For the processing steps feedstock handling, pretreatment and hydrolysis, as well as fermentation, the specific electricity demand has been estimated to increase by a factor of 2. For the remaining liquid processing parts of the plant, the dry feedstock-specific electricity demand has been assumed unchanged. This estimate is considered conservative, increasing the specific electricity demand on a dry feedstock basis for the butanol process by 32%. The heat demand is based on data from³⁷ for the upgrade process of the liquid products and complemented with data for wood-based ethanol production relevant to the current process.³⁸ The demand for chemicals has been increased in relation to the data reported by Tao et al³⁷ for the pretreatment step by a factor of 2 based on Nanada et al⁴⁰ in order to account for the need of harsher pretreatment conditions to achieve comparable yields in downstream hydrolysis when using forest residues as feedstock. Based on data from Nanda et al⁴⁰ the ABE yields from forest residue-based hydrolysates

are similar to those from wheat straw hydrolysate, a comparable feedstock to corn stover. Thus, the ABE yields indicated by Tao et al³⁷ have not been changed. Inventory data for nutrients and chemicals were obtained from the Ecoinvent database. The environmental impact from enzyme production was based on data from the Danish company Novozymes A/C as described in Section 2.3.1.

Similar to the ethanol-based 2-EH pathway, cogeneration of heat and electricity in a CHP plant was assumed using the process by-products (i.e. sludge, biogas & lignin, totaling in 55.5 MW per 100 MW feedstock). Almost 80% of the heat and 90% of the electricity produced are required to operate the ABE fermentation process. The remaining part covers the heat and electricity needs of the butanol to 2-EH conversion step. Excess electricity (1.2 MW) was exported to the grid replacing Swedish average electricity (following the product substitution approach). Besides n-butanol, acetone and ethanol were also produced. Acetone was assumed to replace fossil acetone while ethanol was assumed to replace fossil gasoline. When the RED methodology is applied, butanol was allocated 81% of the upstream impacts on LHV basis.

The conversion of n-butanol to 2-EH was assumed to be nearly complete and the recovery of 2-EH in the downstream purification as high as 99%.

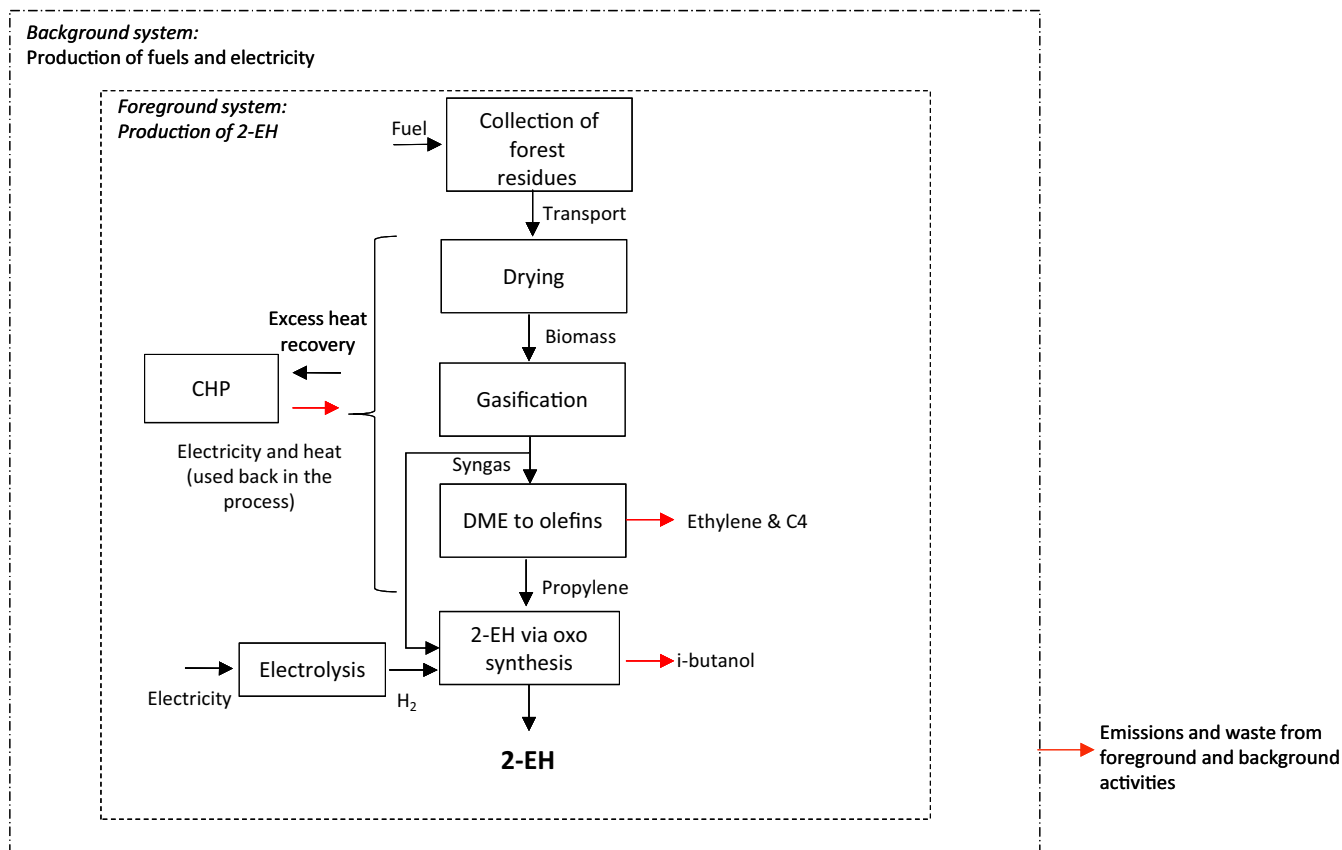


FIGURE 3 2-ethylhexanol production pathway through biomass gasification, obtaining syngas, dimethyl ether and propylene as intermediate chemicals

2.3.4 | Use phase performance of the 2-EH renewable blend

The 2-EH blend considered in the study consists of 43% 2-EH, 50% HVO and 7% RME, which gives a cetane number similar to fossil diesel and can thereby be used in existing diesel engines.¹² The LHV of the blend is 41.1 MJ/kg. The 2-EH blend is used in a mid-sized diesel passenger car. No significant differences in terms of fuel consumption are expected when using this blend according to experimental data from Preuß et al,¹² thus an average fuel consumption of a mid-sized vehicle is considered.⁴¹ As the 2-EH blend consists of 100% renewable content, no carbon dioxide (CO₂) emissions are accounted from fuel combustion according to the methodology applied in the RED.³

2.4 | Environmental impact assessment

The environmental impact of 2-EH was assessed in terms of life cycle primary energy demand and GHG emissions, both being relevant and commonly applied metrics when bioenergy systems are assessed. Water use—being an important indicator for processes based from agriculture-based biomass—has not been considered in the present study as all

processes are based on forest biomass. Primary energy demand (in MJ) was estimated using the Cumulative Energy Demand (CED) indicator. CED considers all energy flows (both renewable and nonrenewable) for energy or materials production,⁴² thus providing a comprehensive analysis of the energy efficiency of the studied system. GHG emissions were assessed as Global Warming Potential (GWP) and expressed in kg of carbon dioxide equivalents (CO₂eq) based on ReCiPe v 1.11.⁴³ The time frame for the assessment was over 100 years. The respective methodologies described in⁴⁴ were followed as applied in OpenLCA v1.7.

3 | RESULTS AND DISCUSSION

3.1 | Environmental assessment of biomass-based 2-EH

The environmental impact of 2-EH produced from renewable feedstock is illustrated in Figures 5 and 6. Figure 5 presents the total primary energy demand as CED for the production of 1 MJ of biomass-based 2-EH. Figure 6 presents the results for the GWP indicator.

Among the three alternative pathways, 2-EH produced through biomass gasification and syngas achieves the lowest

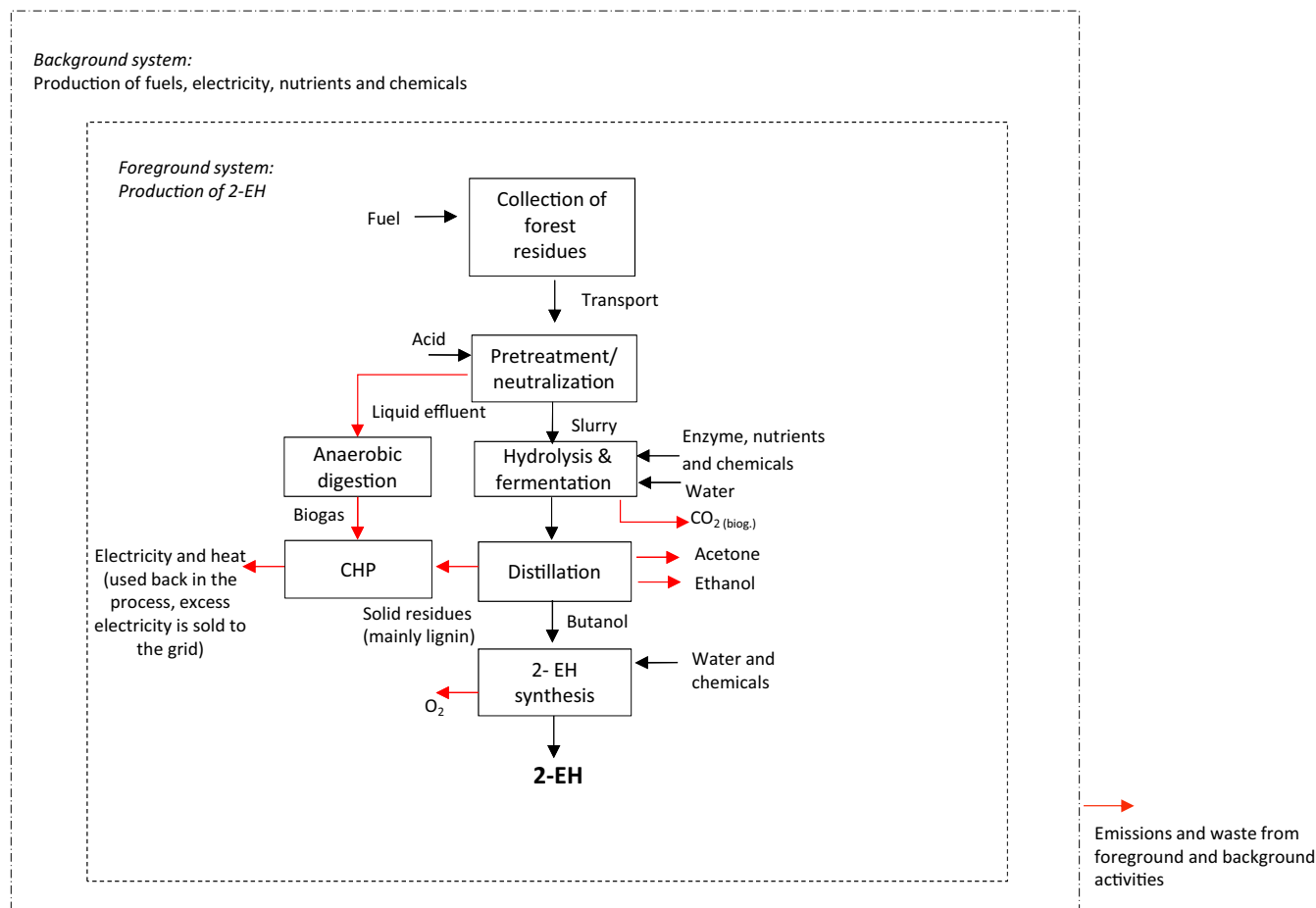


FIGURE 4 2-ethylhexanol production pathway through ABE fermentation, obtaining butanol as intermediate chemical

CED of 3.5 MJ per MJ fuel under the baseline product substitution assumptions, followed by the 2-EH via butanol pathway (3.8 MJ per MJ fuel). 2-EH via ethanol pathway results in the highest CED (4.3 MJ per MJ fuel). When the RED approach is applied, the CED indicator is lower for all pathways, and 2-EH via syngas pathway remains the preferable production route.

A similar pattern is obtained for GWP using the ISO methodology. Due to the possibility to substitute fossil ethylene and butylene during the syngas to olefins conversion process, the net emissions of the gasification pathway are negative, indicating the potential for emissions savings. For the remaining pathways, emissions range between 22 and 35 g CO₂ eq. per MJ 2-EH. When the RED methodology is followed, the GHG emissions from the gasification and butanol pathways are higher. The gasification pathway remains a preferable alternative.

The contribution analysis shows that, for all studied pathways, most of the primary energy demand is a result of feedstock demand (forest residues) thus mostly from renewable resources. Among the three processes, the two biochemical conversion pathways exhibit the highest feedstock to final product (2-EH) efficiency (see also Table 1).

However, these pathways result in high GWP during the biomass conversion steps, mainly due to process materials and chemicals used. For pathway C, the conversion step from butanol to 2-EH contributes to the environmental impact of the fuel to a lower extent, as no hydrogen is needed during the synthesis step. In the case of 2-EH via ethanol and 2-EH via gasification (pathways A and B), 2-EH conversion accounts for 9% and 13% of the CED, respectively, assuming that part of the process energy (such as electricity for hydrogen production) is covered internally. Similar results can be observed for GWP.

Feedstock collection and transport activities are responsible for a minor share of CED for all pathways considered, although they account for the biggest share of nonrenewable energy entering the system (from fossil diesel), thus leading to considerable amounts of GHG emissions. Transport related GHG emissions and the impact on the GWP indicator are highly dependent on the distance and fuel used, which is investigated further in sensitivity analysis.

The results of this work can be compared to a previous study from Patel et al¹⁶ who assessed 2-EH production from ethanol via Guerbet condensation for two scenarios representing current and future conditions, with the latter basically

Cumulative energy demand (CED)

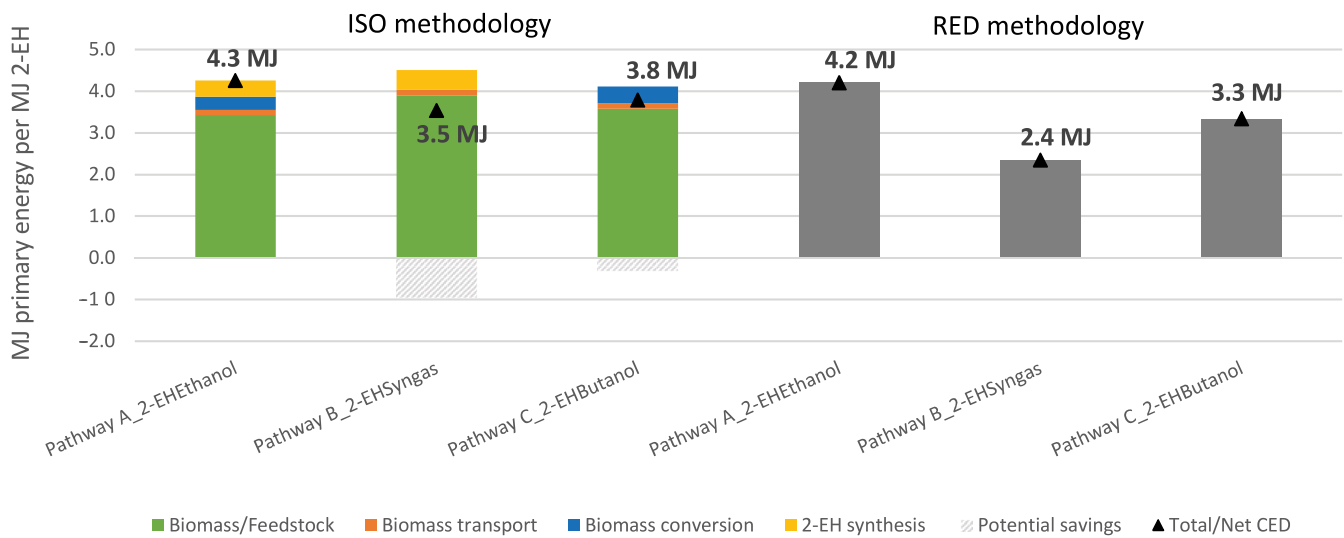


FIGURE 5 Cumulative energy demand for the production of 1 MJ of 2-EH. Left side: results following the ISO methodology (where system expansion and substitution is applied to multifunctional processes). Right side: results following RED methodology (where energy allocation is applied to multifunctional processes)

Global warming potential (GWP)

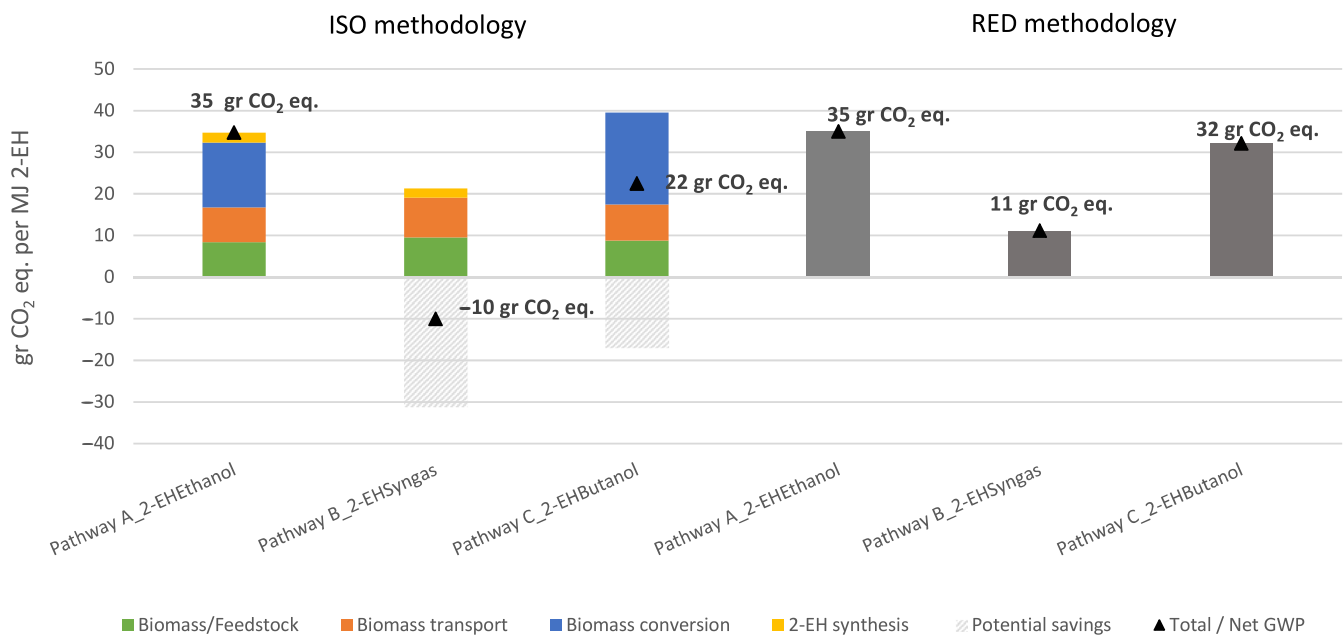


FIGURE 6 Global warming potential for the production of 1 MJ of biomass-based 2-EH. Left side: results following the ISO methodology (where system expansion and substitution is applied to multifunctional processes). Right side: results following RED methodology (where energy allocation is applied to multifunctional processes)

assuming future process improvements with respect to yields and selectivity. Patel et al¹⁶ indicate a CED range of 3.4 to 3.7 MJ/MJ 2-EH and a GWP of 76 to 86 g CO_{2eq}/MJ 2-EH.

The CED is in the same as the results obtained in the present paper whereas the GWP is higher by a factor of about 2 compared to the highest values presented here. The difference can

be due to different LCI data with respect to materials and energy (e.g. ethanol and electricity). It also has to be noted that Patel et al¹⁶ use economic allocation and that the process is different from the pathways analyzed in the present work.

3.2 | Sensitivity analysis

The three pathways considered in this work for the production of 2-EH based on renewable feedstock refers to processes that are not yet commercially available at large scale. Estimations are based on literature and background data which refer to current conditions. Sensitivity analysis is performed aiming to capture process uncertainties such as different ways for by-product handling or supply chain variations (i.e. increased feedstock transport distance) but also process improvements based on likely developments compared to the situation today.

3.2.1 | Alternative scenarios for by-products handling

The ways that by-products are handled can increase or decrease the total amount of externally supplied energy and fuel use, affecting the overall energy and material balance of the system. In the baseline scenarios, it was assumed that heat and parts of electricity demands were covered internally by taking advantage of CHP systems. For the two biochemical pathways exporting internally generated fuels instead of using them for CHP generation is possible whereas for the syngas pathway excess heat is intrinsically used internally. Exporting all biogas and lignin for pathways A and C (and providing electricity and heat by external sources) would increase the total CED of 2-EH production by 17% and 73%, respectively, as shown in Figure 7. The main reason for this increase is the additional biomass input needed for steam generation. In both cases, however, the GWP indicator is decreased if it is assumed that biogas will replace a corresponding fossil alternative such as liquefied natural gas (LNG) in transport applications and lignin is exported to a power plant and the power replaces average Swedish electricity (assuming a power plant efficiency of 0.4). If a more carbon intense electricity mix is replaced (such as the average European electricity mix with a carbon intensity of 134 g CO_{2eq} per MJ_{el}⁴⁵) the overall GWP savings are greater (see Figure 7). This could represent a situation where the production facility is located outside Sweden and in countries where the electricity mix is dominated by fossil resources such as coal or natural gas.

3.2.2 | Alternative scenarios in relation to feedstock transport

As discussed above, transportation of biomass from the collection point to the fuel production facility results in considerable

GHG emissions in all baseline scenarios. The GWP related to the transport of feedstock could therefore be decreased if renewable fuels are used. If biodiesel is assumed for feedstock transportation (instead of fossil diesel), GWP for 2-EH production can be reduced by 17% for the ethanol production pathway, and 60% and 27% for the syngas or butanol-based pathways respectively (see Figure 8). CED increases by 2.5%–6%, since biodiesel requires more primary energy than conventional diesel. However, as fossil primary energy is substituted with renewable sources, the total share of fossil primary energy during 2-EH production is also reduced significantly.

Variations in feedstock transport distance influence the overall GWP impact of 2-EH. By doubling the distance (to 600 km), the overall impact increases by 18% for ethanol based 2-EH (in the baseline scenario), 28% for butanol based 2-EH, whereas for 2-EH produced via syngas, the total GHG emissions are doubled (thus the values are close to zero in Figure 8). Decreasing transport distance, on the other hand, reduces not only energy demand but most importantly GHG emissions from 15% to 24% depending on the 2-EH production pathway considered.

3.2.3 | Process improvement scenarios

Finally, process improvements in relation to current systems were explored for all three studied pathways assuming:

- 10% increase of 2-EH yield assuming improved selectivity; overall conversion efficiency from biomass to products remains unchanged so by-products' yields are reduced correspondingly.
- 10%-points increase of the electricity to hydrogen efficiency rate (from 0,65 to 0,75 MJ_{H₂LHV}/MJ_{el}) reducing the total amount of energy needed during the 2-EH conversion step.
- 50% reduction of the enzyme-related environmental impact during the fermentation processes (in the short to medium term i.e. by 2022) as a result of process optimization efforts and improved enzyme activity.²⁹ These assumptions are valid only for the two biochemical conversion pathways (A and C).

The resulting mass and energy balances considered are shown in Table 2.

Based on these assumptions, the primary energy demands of 2-EH production can be reduced for all pathways as shown in Figure 9. However, only 2-EH production via ethanol benefits from GHG emissions reductions of about 15%. In the two remaining pathways (B and C), GHG emissions increase, which are a result stemming from that by-products typically contribute very well to the total GHG-reduction when they substitute existing equivalent products. As by-products' yields decline, the impact reduction potential from product substitution declines as well.

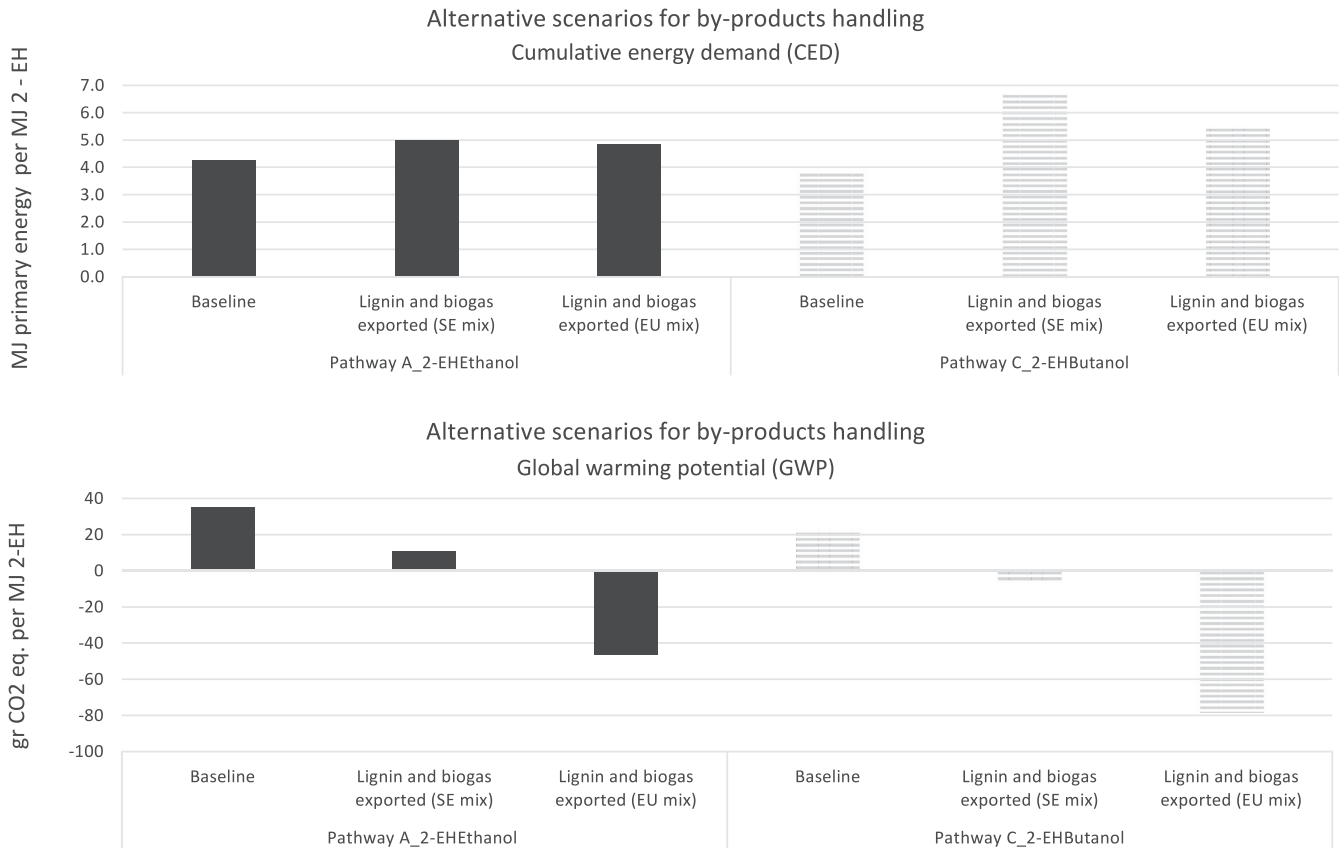


FIGURE 7 Alternative scenarios for by-product handling of the two biochemical conversion pathways. The figure illustrates the CED (top) and GWP (bottom) indicators when the ISO methodology is assumed

3.3 | Comparison of the 2-EH blend to fossil and renewable transportation fuel alternatives

In order to provide a rough benchmark of this novel fuel and compare it to existing fossil and renewable alternatives the WTW performance of a 100% renewable fuel blend consisting of 43% 2-EH, 50% HVO and 7% RME is estimated, where impacts from both fuel production and consumption are considered.

The environmental impact from 2-EH production was based on the baseline scenarios presented above (Figures 5 and 6). The environmental performance of tall oil-based HVO was reestimated by the authors based on a previous study from Becker et al⁴⁶ to be 2.54 MJ/MJ HVO and 6.1 g CO_{2eq}/MJ HVO. For RME, data were taken directly from Edwards et al³³ (1.91 MJ/MJ RME and 47 g CO_{2eq}/MJ RME). By taking into consideration the share of each constituent, the total CED of the blend was estimated to be in a range of 2.9–3.2 MJ/MJ blend depending on the production process for 2-EH. Although these values are almost three times higher than fossil diesel (1.2 MJ/MJ fuel³³) they are close to the primary energy requirements of other renewable fuels such as ethanol (2.3–3.1 MJ/MJ fuel).³³ When GWP is concerned, the impact

from fuel's production range from 3 g CO_{2eq}/MJ blend (when 2-EH via syngas is assumed) to 21 g CO_{2eq}/MJ blend when 2-EH is produced via ethanol.

Taking into consideration fuel consumption during use phase, the WTW CED of the 2-EH blends ranges from 5.1–5.3 MJ/km. Regarding GWP, the WTW impact of the 2-EH blends range from 4.6 to 36 g CO_{2eq}/km. Figure 10 illustrates the comparison between the 2-EH blend (produced via different pathways) and existing fossil and biomass-based fuels. All data (except for the 2-EH blends and HVO [from tall oil]) are based on the study by Edwards et al⁴¹ for consistency reasons and due to similarities in terms of methodological approach (following the product substitution principle).

As shown in Figure 10, the 2-EH blends exhibit the highest CED than most existing fuels. An increase in primary energy demand can be expected due to additional conversion steps.

However, when GWP is concerned 2-EH blends provide clearly a preferable fuel compared to fossil diesel. Due to the renewable nature of the fuel constituents, the 2-EH blends result to no fossil CO₂ emissions during the use phase. WTW GHG emissions can therefore be reduced by 85%–98% compared to fossil diesel depending on the

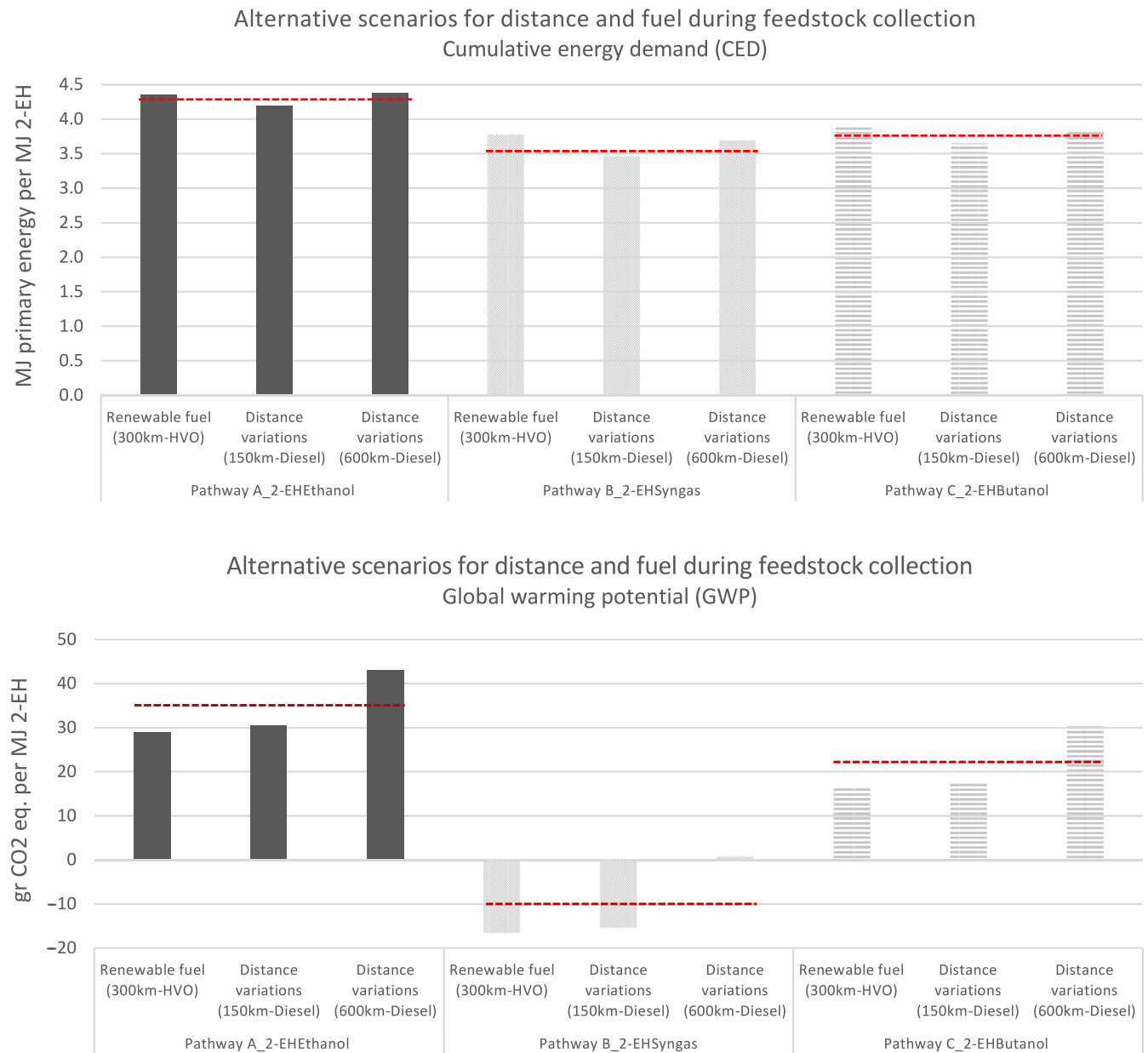


FIGURE 8 Alternative scenarios for fuel and distance during feedstock collection and transport process. Figure illustrates the CED (top) and GWP (bottom) indicators when the ISO methodology is assumed. The red lines represent the respective baseline scenarios where fossil diesel and a distance of 300 km are considered as default values

2-EH production pathway. These savings are well above the 60% requirements set by the RED and can be comparable to other second generation biofuels such as ethanol, methanol, HVO etc. that exhibit GHG emissions savings from 80%-96%.⁴⁶

As illustrated in Figure 10, 2-EH blends perform better in relation to some biofuel alternatives such as Ethanol85, neat biodiesel (RME) as well as neat HVO (from tallow oil) while the GWP of the blend containing 2-EH produced via biomass gasification (pathway B) is comparable to fuels such as DME despite the additional conversion steps involved.

3.4 | Fuel supply considerations

More than 80% of primary energy for 2-EH production comes from renewable sources, the majority of which relates to the biomass needed as feedstock. Although indirect land use conflicts are avoided using forest-based residues, the widespread adoption of 2-EH as alternative transport fuel could nevertheless be hindered by feedstock availability.

The demand for biomass is expected to increase across different sectors as EU countries have committed to increase their renewable energy share. Sweden depends highly on bioenergy and has one of the highest shares of renewable

TABLE 2 Energy balance (LHV basis) during 2-ethylhexanol production under the studied process improvement scenarios

		2-EH Production pathways		
		2-EH _{Ethanol}	2-EH _{Syngas}	2-EH _{Butanol}
Input	Biomass (50 wt-% m.c. forest residues)	100 MW	100 MW	100 MW
	Electricity import	4.1 MW	0.2 MW	–
Main product	2-EH	37.2 MW	30.2 MW	36 MW
	Excess electricity	–	–	0.7 MW
	Ethylene (C ₂)	–	17 MW	–
	Butylene (C ₄)	–	8 MW	–
	i-butanol	–	1.3 MW	–
	Acetone	–	–	0.9 MW
	Ethanol	–	–	2.9 MW
Efficiency metrics	n_{bio} (biomass to 2-EH)	37.2%	30.2%	36%
	n_{tot} ($n_{\text{out}}/n_{\text{in}}$)	35.8%	56.5%	40.4%

fuels for transport in the EU.⁴⁷ In 2016, approximately 18% (17 TWh) of the road transport energy demand in Sweden was covered by bio-based fuels, mostly in form of biodiesel, ethanol and biogas,⁴⁸ produced to a large extent from agricultural crops.⁴⁹ To meet the national emission reduction targets for the transport sector, the Swedish government expects that by 2030, 50% of petrol and diesel vehicles will run on bio-based fuels.⁵⁰ To achieve that goal, taking into consideration the restrictions posed by the revised renewable energy directive (RED II) regarding crop-based fuels, the demand for alternative and sustainably produced biogenic feedstock can be expected to rise. Börjesson et al⁴⁹ have estimated an increase in the Swedish demand for forest biomass for biofuels production of 18–20 TWh per year until 2030, which corresponds to a 160%–180% increase compared to current conditions. With a simultaneous increase in forest-based biomass demand in other sectors (such as the chemical industry) there is a high risk that domestic supply will not be sufficient to cover the expected demand.^{49,51} This stresses the need for optimized production processes and the implementation of additional energy efficiency measures that would enhance the use of biogenic feedstock across different sectors.

4 | CONCLUSIONS

“Drop-in” renewable fuels can contribute significantly towards reducing GHG emissions in the transportation sector in the short to medium term by taking advantage of existing infrastructure both when motor engines and fueling systems are concerned. A novel fuel, 2-ethylhexanol, has been investigated in this work and assessed from a life cycle perspective. The study presented three different pathways for 2-EH production based on renewable feedstock which also

provided different opportunities for a reduction of GHG emissions when by-products substitute existing equivalent products.

The total CED of 2-EH was shown to be in the range of 3.5–4.3 MJ/MJ 2-EH with potential for improvement when optimized processes are in place. As expected those values are slightly higher than existing biomass-based renewable fuels since additional conversion steps are added to the production chain. The conversion step from intermediate to final product accounts for 9% and 13% of the total CED for the ethanol and syngas pathways, respectively, mainly due to the use of hydrogen. For the butanol pathway, the impact of the final conversion to 2-EH is significantly lower both from a GWP and CED perspective. With respect to GWP, 2-EH production via syngas and butanol benefits to a large extent of effects of by-products substituting fossil alternatives. This is in particular true for the syngas pathway. Improvement in 2-EH yield at the cost of by-product yield decreases the GWP performance of 2-EH via syngas and butanol, but improves it for 2-EH via ethanol, where only internal fuels are generated as by-products. The export of internally generated fuels—e.g. biogas and lignin—for electricity generation for the two biochemical 2-EH pathways leads to increased CED and decreased GWP. The positive effects of decreased GWP are more pronounced for carbon-intensive electricity markets.

From a WTW perspective, 2-EH was shown to be a promising fuel. A fully renewable fuel blend containing 2-EH has a WTW GWP comparable to that of DME and HVO (from tall oil). In particular, the gasification-based WTW emissions are competitive with e.g. DME, 2-EH having the advantage of being a drop-in fuel with high blending potential. Full-scale adoption of DME requires substantial modifications in terms of drivetrain and fuel distribution infrastructure, and

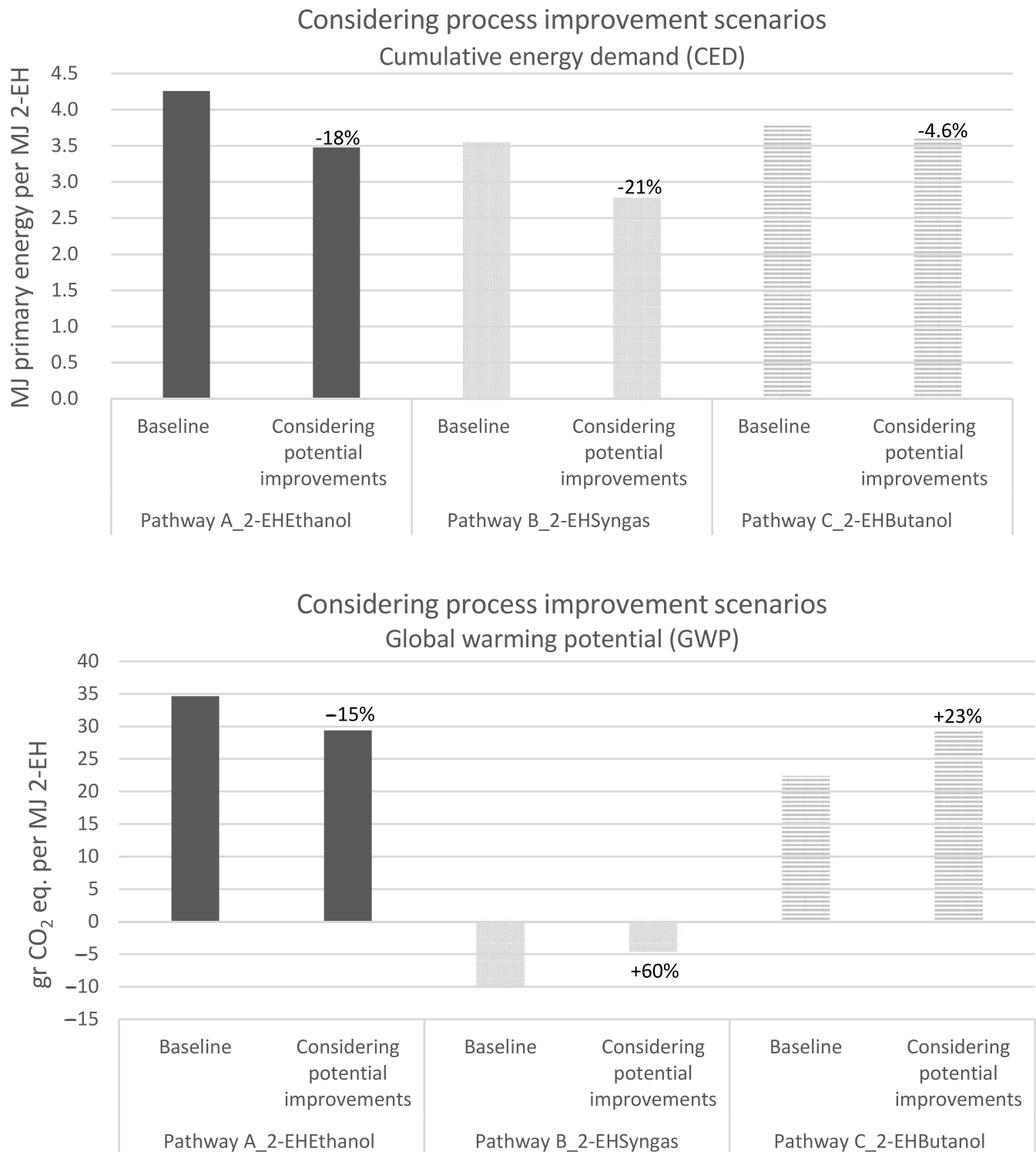


FIGURE 9 Impact of selected improvements to the 2-ethylhexanol production process. Impact on CED (top) and GWP (bottom) indicators when the ISO methodology is applied

tall oil-based HVO faces feedstock availability challenges. 2-EH used in renewable blends could be therefore considered a promising short- to medium-term alternative for increasing the biofuel share of the transport sector. This, in combination

with lower regulated emissions during combustion, as measured in previous experimental work, make 2-EH a competitive fuel that could further enhance the efforts for minimizing local air pollution.

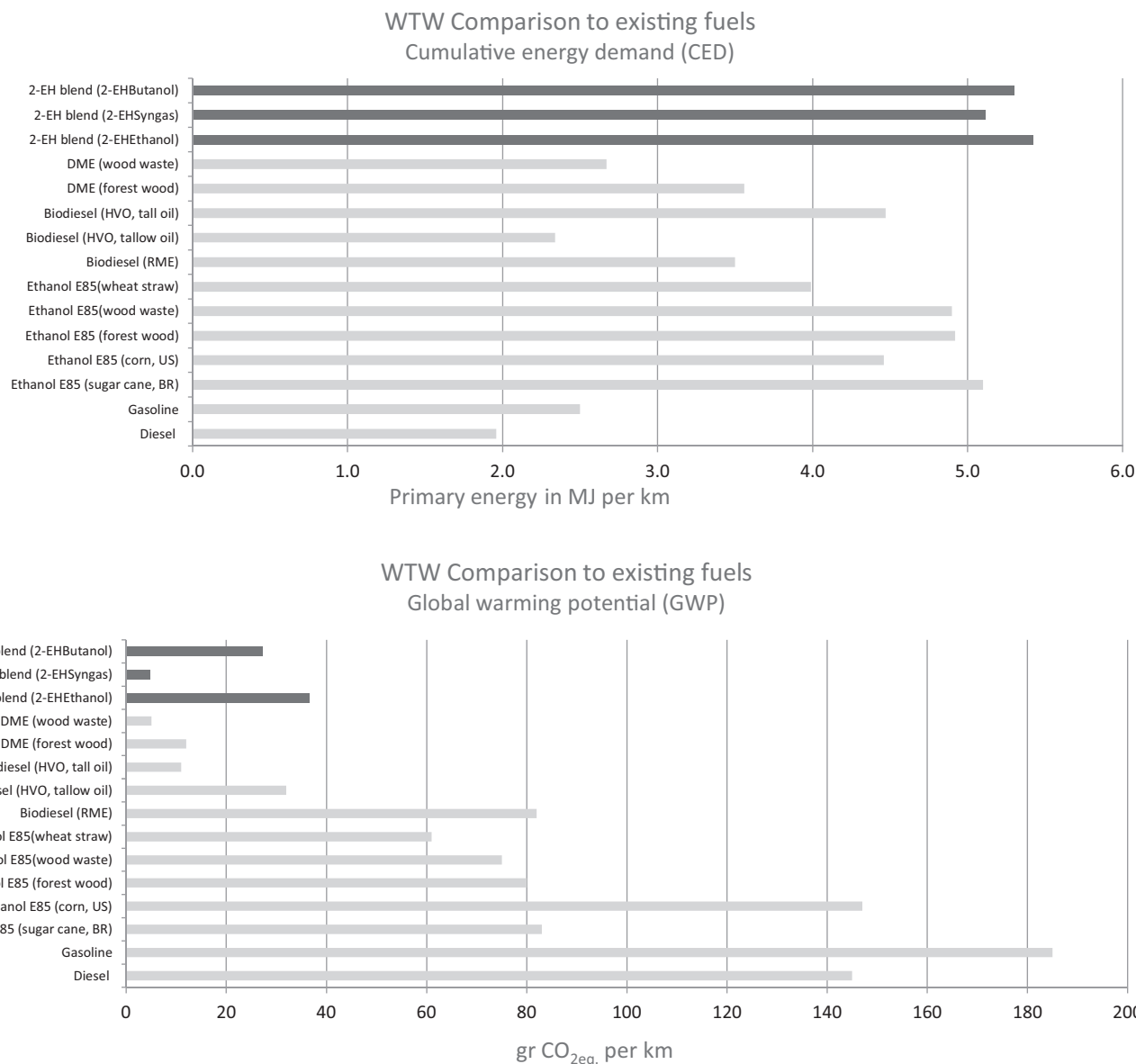


FIGURE 10 Well-to-wheel CED (top) and GWP (bottom) of different bio-based and fossil fuels used in a passenger car. All data are from Edwards et al.⁴¹ except for the 2-ethylhexanol blend (43% 2-EH, 7% RME (from rapeseed) and 50% HVO (from tall oil))

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