Hydroformylated Fischer-Tropsch Fuels for Sustainable Transport

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Abstract: The use of synthetic fuels has shown high potential to achieve sustainable transportation. However, the current synthetic fuel options are either not suitable for the current fleet of vehicles or require new production processes, which has delayed their introduction to the market. A potential solution is the use of Hydroformylated Fischer-Tropsch (HyFiT) fuels. This fuel option combines two established technologies, Fischer-Tropsch synthesis and hydroformylation, to create a mixture of alkanes and alcohols that can serve as fuel. The goal of HyFiT-fuels is to address four main challenges of synthetic fuels: (1) using mature technologies, (2) compatibility with global fuel standards and elastomer materials, (3) reducing combustion-induced emissions, such as nitrogen oxides (NO_X) and particulate matter (PM), and (4) supporting the transition to net-zero greenhouse gas emissions. The research conducted shows that HyFiT-fuels can effectively tackle all of these challenges simultaneously, and therefore, offer a promising complement to electrification efforts.

The investigations reveal the potential of HyFiT-fuels with 20 and 40 wt% alcohol content (HyFiT-20% & HyFiT-40%) to replace diesel fuel in a light commercial hybrid electric vehicle. The study experimentally examines the fuel's impact on the emissions of CO_2, PM, and NO_X, and the theoretical potential for NOx reduction by increasing exhaust gas recirculation (EGR) rates. The results show that HyFiT-fuels used as drop-in fuel without any further adaptations can reduce PM engine-out emissions by 55% (HyFiT-20%) respectively 70% (HyFiT-40%) and CO_2 tailpipe emissions by 3-5% compared to diesel fuel.

1 Introduction

In 2021, approximately 740 million metric tons of carbon dioxide (CO_2) were emitted in the EU due to the combustion of fuels in road transportation. Passenger cars and motorcycles were responsible for the majority of these emissions, accounting for 64 %. Trucks and buses contributed 27 %, while light commercial vehicles made up the remaining 10 %. Despite efforts to reduce emissions in recent years, progress has been limited. Although improvements in engine technology, exhaust aftertreatment systems, and the use of new fuels such as RON 95 E10 have helped reduce pollutant emissions, these measures have been outweighed by the rising volume of traffic and an increasing number of highly motorized vehicles with relatively high fuel consumption. Between 1990 and 2021, annual CO_2 emissions from road transportation in the EU increased by 21 %. The most significant increase was observed in light commercial vehicles, with a 49 % rise in CO_2 emissions. CO_2 emissions from trucks and buses grew by 28 %, while those from passenger cars increased by 15 %. To achieve climate neutrality by 2050, the EU aims to make significant strides with the European Green Deal. [EEA23]

A crucial strategy for mitigating GHG emissions and alleviating urban air pollution entails the combination of renewable energy generation with the direct electrification of the transportation sector. However, certain segments of the transportation that are challenging to electrify, such as aviation, shipping, and trucks, may continue to rely on liquid energy carriers in the foreseeable future. For these specific transport sectors, the transition from fossil-based to clean, bio-based, and electricity-based synthetic fuels offers a promising solution to reduce GHG emissions and combat urban air pollution.

Synthetic fuels offer advantages due to their compatibility with existing infrastructure for liquid energy carriers and their ability to indirectly incorporate renewable energy into the transportation sector by utilizing renewable sources for fuel production. This can include harnessing renewable energy from regions abundant in wind and solar resources, such as Chile, Australia, North Africa, and Middle Eastern countries.

However, synthetic fuels are facing four main challenges: (1) using mature technologies, (2) compatibility with global fuel standards and elastomer materials, (3) reducing combustion-induced emissions, such as nitrogen oxides (NO_X) and particulate matter (PM), and (4) supporting the transition to net-zero greenhouse gas emissions.

A comprehensive study including the production process & fuel design, material compatibility investigations up to combustion emissions measurements and a subsequent, comparative well-to-wheel Life Cycle Assessment (LCA) reveals that Hydroformylated Fischer-Tropsch (HyFiT) fuels, a combination of two established technologies, Fischer-Tropsch (FT) synthesis and hydroformylation, can effectively tackle all of these challenges simultaneously [Sim24]. This article gives a more detailed impression of the vehicle tests carried out as part of this study and highlights the potential for greenhouse gas and pollutant emission savings on a tank-to-wheel basis.

2 Hydroformylated Fischer-Tropsch (HyFiT) Fuels

The HyFiT-fuel production concept consists of several process units including FT synthesis and hydroformylation. Depending on the FT synthesis, the resulting HyFiT-fuel is either rich in alkanes (C5 to C17) or alcohols (C6 to C11), so that the desired alcohol-alkane ratio of the HyFiT-fuel can be adjusted. The alcohol percentages of 20 and 40 wt% (HyFiT-20% & HyFiT-40%) were selected for the vehicle tests, as these cover a reasonable range of minimum tolerable viscosity with high cetane number at 20 wt% and minimum acceptable cetane number at 40 wt%. The fuel properties of the two mixtures can be found in Table 1. To comply with the lubricity limits of max. 460 µm (EN590), 2000 ppm of R655 have been added. An influence on the other characteristic values could not be observed.

Table 1: Fuel properties of HyFiT fuels with 20 and 40 wt% alcohol content [Sim24]

		HyFiT-20%	HyFiT-40%
Lower Heating Value	MJ kg^{-1}	42.9	41.5
Derived Cetane Number	-	64	56
Viscosity	mm^2s^{-1}	1.5	2.0
Lubricity (HFRR[1])	µm	568	546
		430[2]	430[2]

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[1] High Frequency Reciprocating Rig

[2] Measured with additive: 2000 ppm of R655

3 Vehicle Powertrain Layout and Testing Boundary Conditions

The demonstration vehicle is categorized as a light commercial vehicle (LCV). It is equipped with a 4-cylinder 2.0 L internal combustion engine (ICE) boasting a rated power of 130 kW, featuring high-pressure (HP) exhaust gas recirculation (EGR). The vehicle's exhaust aftertreatment system (EATS) includes a diesel oxidation catalyst (DOC), a diesel particulate filter (DPF) with a selective catalytic reduction (SCR) coating (SCRF), functioning both as DPF and SCR, and an ammonia slip catalyst (ASC). Both the engine and the exhaust aftertreatment system of the vehicle underwent certification in accordance with heavy-duty standards (EU VI D).

For demonstration purposes, the conventional vehicle underwent a transformation into a high voltage full hybrid electric vehicle, completed with an automatic 8-gear transmission. The hybrid powertrain configuration adopted is denoted as P0P2, as illustrated in Figure 1. Although the electric motor placed in the P0 position for enabling the ICE's On/Off switching, the hybrid powertrain predominantly functions as a P2 hybrid. Essential specifications of the hybrid powertrain are summarized in Table 2. Further details regarding the hybrid demonstrator's configuration and its operational features can be found in [Sch20a] and [Sch20b].

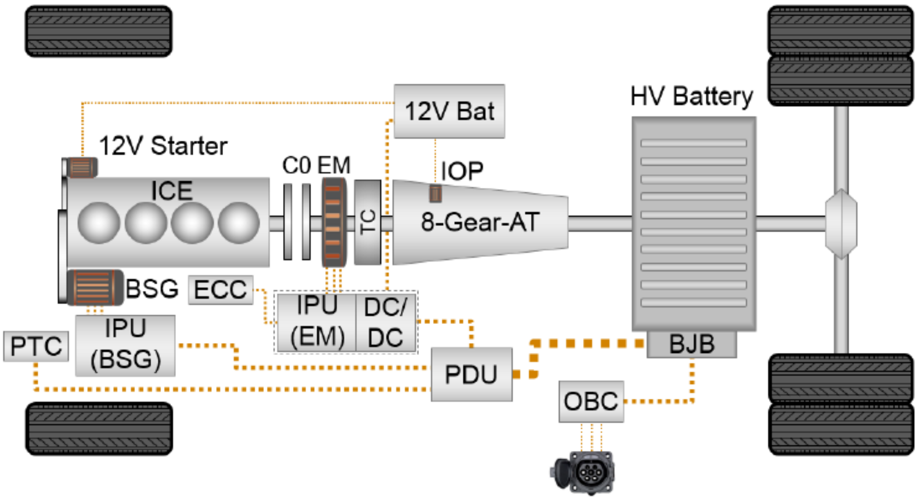


Figure 1: Powertrain layout of the hybrid electric LCV demonstrator

Table 2 : Electric components of the hybrid electric LCV demonstrator

		P0P2-HEV
EM (Electric Machine) Power	kW	60 (cont.) / 95 (peak)
EM Type	-	PMSM
Li-Ion Battery Capacity	kWh	14
Nominal System Voltage	V	310

During each test, the total vehicle weight remained constant at 3.3 metric tons. As per regulations, carbon dioxide (CO_2) emissions for vehicles with a total mass below 3.5 metric tons, falling under the N1 category, are certified in accordance with the Worldwide Harmonized Light Vehicle Test Cycle (WLTC) standards [RegEU19]. The WLTC is designed to emulate the typical driving patterns of both passenger cars and vans across Europe. Forming part of the pollutant emissions certification process for light-duty vehicles next to the Real Driving Emissions (RDE) testing requirements, which were introduced within the EU6d-temp regulatory framework, the WLTC is commonly employed for emission calibration.

Given that the vehicle is used as a truck with a speed limit of 120 km/h for safety considerations, the WLTC120 was selected as the appropriate testing cycle for the experimental campaign. All measurements were conducted at an ambient temperature of 23 °C and with a consistent overall vehicle mass of 3.3 metric tons, under charge sustain State of Charge (SoC) conditions. Prior to each test, activities such as the regeneration of the SCRF and its pre-loading with ammonia (NH_3) were carried out. These procedures were performed to establish uniform boundary conditions, ensuring a valid and equitable comparison of the emission measurements across all tests.

4 Engine-Out and Tailpipe Emissions Performance of HyFiT Fuel as Drop-In

Figure 2 provides a summary of the WLTC120 emission measurements for a) carbon dioxide (CO_2), d) particulate matter (PM) and e) & f) nitrogen oxides (NO_X). Vehicle hardware as well as calibration has been kept unchanged characterizing the fuel variation as “drop-in”. As previously indicated, all emissions measurements have been adjusted for ΔSoC variations across the entire test cycle to ensure a consistent basis for comparison. Figure 2 b) illustrates the ΔSoC deviations and the corresponding additional CO_2 emissions observed between the initial SoC and the final SoC for each test case. This variation can be attributed, on one hand, to driver influences and, on the other hand, to the fuel change, both of which contribute to a slight difference in power distribution between the Internal Combustion Engine (ICE) and the Electric Motor (EM). Consequently, this results in a minor variance in the amount of battery energy utilized within the system over the entire cycle.

Furthermore, an empirically determined 2 % increase in CO_2 emissions over the entire WLTC120 cycle is factored in for the fossil Diesel case to account for Diesel Particulate Filter (DPF) regeneration events that occur in real-world street operations. To accommodate the less frequent need for regeneration events when utilizing HyFiT fuels, owing to their significantly reduced engine-out soot emissions, the CO_2 increase is proportionally scaled down based on the decrease in engine-out soot emissions observed in the HyFiT cases compared to fossil Diesel (see Figure 2 c)).

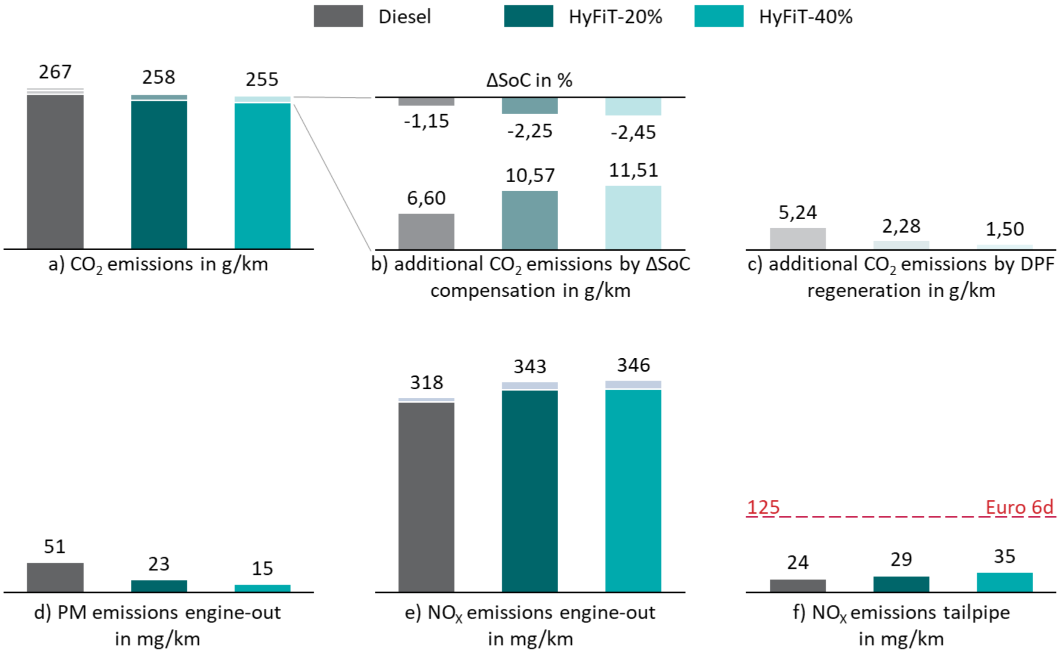


Figure 2: cumulative a)-c) carbon dioxide (CO_2), d) particulate matter (PM) and e)-f) nitrogen oxides (NO_X) emissions during WLTC120 of Diesel, HyFiT-20% and HyFiT-40% fuels as Drop-In

Based on the findings presented in Figure 2, we observe an approximate 3 % reduction in carbon dioxide (CO_2) emissions with HyFiT-20% and about a 5 % reduction in CO_2 emissions with HyFiT-40%, as compared to fossil Diesel. This decrease can be attributed to the higher oxygen content of both HyFiT fuels. In terms of engine-out soot emissions, there is an approximately 55 % reduction with HyFiT-20% and an approximately 72 % reduction with HyFiT-40%, again owing to the increased oxygen content.

Regarding nitrogen oxides (NO_X) emissions, we note that engine-out NO_X emissions are approximately 8 % higher for HyFiT-20% and approximately 9 % higher for HyFiT-40% when compared to fossil Diesel. It is essential to highlight that the influence of the different fuels on tailpipe NO_X emissions appears more pronounced than on engine-out NO_X emissions. This is attributed to the combined effects of both higher engine-out emissions and the delayed exhaust aftertreatment system (EATS) heat-up on the tailpipe NO_X emissions. Consequently, tailpipe NO_X emissions seem to be around 24 % higher for HyFiT-20% and approximately 48 % higher for HyFiT-40% when compared to fossil Diesel.

Notably, for increased vehicle speed at the end of the WLTC120 a substantial increase in engine-out NO_X emissions followed by a modest increase in tailpipe emissions were observed during the WLTC using HyFiT fuels. This increase can be primarily attributed to the non-optimized urea dozer strategy of the SCRF, which is calibrated based on Diesel fuel properties. However, it's essential to emphasize that EATS optimization for the HyFiT fuels falls outside the scope of the current study and was not further investigated.

The HyFiT fuels have effectively demonstrated their Drop-In compatibility and have shown advantages in terms of reducing both CO_2 and soot emissions. The relatively poorer tailpipe NO_X performance can be attributed to the fact that the internal combustion engine (ICE) and exhaust aftertreatment system (EATS) calibration were not optimized for HyFiT fuels. In a comprehensive vehicle calibration process, both the ICE and the Selective Catalytic Reduction (SCR) control strategy would be adjusted to align with the combustion characteristics of the new fuel. However, it is worth highlighting that the tailpipe NO_X emissions performance of the HyFiT fuels, even though it surpasses that of fossil Diesel, still falls below the current EU6d legislation (125 mg/km).

5 Exploiting the Emission Reduction Potential of HyFiT Fuels

In the following section, the authors aim to showcase the full emission reduction potential achievable by promptly implementing the examined HyFiT fuels as Drop-In substitutes in the existing fleet combined with a potential improvement by an optimized calibration. Through a theoretical investigation, the substantial advantages of HyFiT fuels in reducing engine-out soot emissions by as much as 70 % will be leveraged to estimate the potential reduction in overall tailpipe NO_X emissions.

The approach comprises three steps. In the initial step, the emissions performance of both HyFiT and Diesel fuels is compared at specific characteristic operating points (OPs) aligned with the operational profile of the LCV demonstrator during the WLTC. Following this, the observed trends are extrapolated to powertrain level using simulation. In this step, the engine-out emissions recorded during the transient tests with HyFiT fuels are adjusted to model two distinct low-NO_X internal combustion engine (ICE) calibration scenarios, derived from previous Single Cylinder Engine measurements. Finally, the tailpipe emissions are ultimately predicted for the engine-out emissions optimized for low-NO_X, incorporating assumed efficiencies for the individual exhaust aftertreatment system (EATS) components.

As shown in [Neu18], depending on the permissible limit of soot emissions and the calibration of in-cylinder anti-pollution measures, such as high exhaust gas recirculation (EGR) strategies and retarded injection, hydroformylated Fischer-Tropsch fuels can enable indicated specific NO_X levels as low as 0.1 g/kWh. This advantage offered by oxygenated fuels can also be leveraged to mitigate tailpipe NO_X emissions. Nonetheless, it's important to acknowledge that in-cylinder anti-pollution measures come with trade-offs that negatively affect CO_2 emissions. Consequently, such a low-NO_X mode should only be engaged under specific operating conditions where the exhaust aftertreatment system (EATS) cannot achieve high conversion efficiencies, like during warm-up. Here, the low-NO_X mode of HyFiT fuels is explored until the SCRF reaches its designated operating temperature range of approximately 200°C after 825 seconds. Beyond this point, the SCRF can effectively convert nearly all engine-out NO_X emissions, resulting in virtually negligible tailpipe NO_X emissions.

Two scenarios for an optimized HyFiT engine calibration where modelled:

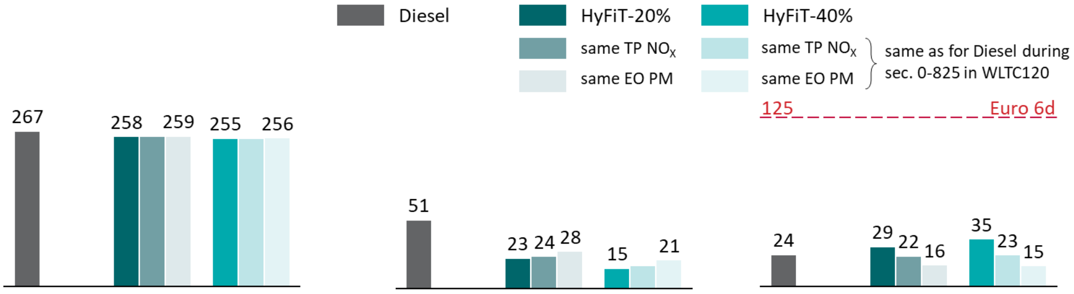
a) A scenario in which, during the initial 0-825 seconds phase, the engine-out soot emissions of the HyFiT fuels match those of fossil Diesel

b) A scenario in which, during the initial 0-825 seconds phase, the tailpipe NO_X emissions of the HyFit fuels match those of fossil Diesel

The first scenario illustrates the theoretical maximum potential for NO_X emissions reduction, which concurrently results in a maximum increase in engine-out soot emissions, reaching levels akin to those of the fossil Diesel case. In the second scenario, the necessary engine-out NO_X emissions level is estimated to ensure equivalent tailpipe NO_X emissions with fossil Diesel. It's important to note that after approximately 825 seconds, the vehicle's SCR system reaches its desired operating temperature range, rendering low-NO_X measures unnecessary. For the purposes of this study, the emissions level in the phase beyond 825 seconds is assumed to remain constant and equivalent to the measured Drop-In emissions.

Figure 3 provides a comprehensive overview of all emissions results, accounting for the ΔSoC correction and DPF regeneration in all cases. According to the results, both HyFiT fuels exhibit lower CO_2 emissions when compared to fossil Diesel. This trend persists even when the HyFiT-dedicated low-NO_X calibration is implemented, albeit with a minor drawback compared to the pure Drop-In scenario. Likewise, in all cases involving HyFiT fuels, engine-out soot emissions are notably reduced in contrast to the case of fossil Diesel.

Based on the simulation studies, leveraging the full potential for reducing engine-out NO_X emissions with HyFiT fuels can result in a remarkable up to 35 % reduction in tailpipe NO_X emissions over the entire WLTC120 in comparison to fossil Diesel. This reduction can be attributed to the significantly lower level of engine-out NO_X emissions achieved before the Selective Catalytic Reduction Filter (SCRF) light-off is reached, compensating for the limited de-NO_X capacity of the system during this phase. As for tailpipe soot emissions, the DPF effectively filters nearly 100 % of the emitted soot in all cases, resulting in almost negligible tailpipe soot emissions and are therefore not shown here.



a) CO_2 emissions in g/km

b) PM emissions engine-out (EO) in mg/km

c) NO_X emissions tailpipe (TP) in mg/km

Figure 3: cumulative a) carbon dioxide (CO_2), b) particulate matter (PM) and c) nitrogen oxides (NO_X) emissions during WLTC120 of Diesel, HyFiT-20% and HyFiT-40% fuel with optimized calibration for emission reduction

As a result, the HyFiT-dedicated low-NO_X strategies do introduce certain disadvantages related to CO_2 and engine-out soot emissions. Nonetheless, these drawbacks can be offset on one hand by the substantial reduction in tailpipe NO_X emissions and on the other hand by the efficient functioning of the Diesel Particulate Filter (DPF), which ensures zero tailpipe soot emissions.

6 Conclusions

In conclusion, our extensive vehicle measurement campaign has effectively assessed the drop-in compatibility of HyFiT fuels within the WLTC120 framework. Our tests have verified that these E-Fuels can seamlessly enable the same vehicle drivability as fossil Diesel. Furthermore, we identified a noteworthy CO_2 reduction benefit of up to 5 %. The standout feature of HyFiT fuels lies in their significant reduction of engine-out soot emissions by a remarkable 50-70 %, which can serve as a valuable counterbalance to the downside of increased tailpipe NO_X emissions. It's worth noting that even with the immediate implementation of HyFiT fuels, we observed no violation of the stringent EU6d NO_X limits in the WLTC120, underscoring the neutrality of HyFiT fuels in terms of air quality impact, as defined by regulatory vehicle emissions standards.

However, the HyFiT-fuels produce slightly higher NO_X engine-out emissions of around 8-9 %, resulting in higher NO_X tailpipe emissions for HyFiT-20% (29 mg/km) and HyFiT-40% (35 mg/km) than for diesel (24 mg/km).

Utilizing the exceptionally low engine-out soot levels achievable with HyFiT fuels, it becomes possible to substantially reduce tailpipe NO_X emissions to levels significantly below those of fossil Diesel without burdening the Diesel Particulate Filter (DPF). Through the implementation of HyFiT-dedicated low-NO_X strategies, the remarkably low engine-out emissions during these phases can offset the limitations of the Selective Catalytic Reduction (SCR) efficiency until the required temperature is reached. This, in turn, leads to an overall reduction in tailpipe NO_X emissions, particularly in areas characterized by emissions related to the cold exhaust aftertreatment system. In this study, a 35 % reduction in tailpipe NO_X emissions over the entire WLTC120 in comparison to fossil Diesel was observed.

Given that HyFiT fuels are drop-in capable, these measures can be readily integrated into the existing vehicle fleet through minor adjustments in the internal combustion engine calibration, provided that the vehicle powertrain hardware can accommodate these adaptations.

Looking ahead to the future of vehicle fleets, the insights from our study can be pivotal in shaping the EU7 technology package for vehicle manufacturers. An optimized HyFiT-dedicated low-NOx strategy has the potential to downsize both the de-NOx unit and the DPF, resulting in cost savings and improved ICE efficiency by reducing EATS-induced backpressure. Furthermore, the exceptional capability of HyFiT fuels to limit engine-out NOx emissions during cold starts can obviate the need for additional heating devices in the EATS, such as electrical heaters.

In conclusion, the benefits of HyFiT fuels extend beyond their contribution to achieving "net-zero" CO_2 emissions. They also hold promise for enhancing air quality impacted by the transportation sector. Consequently, HyFiT fuels, and fuels based on renewable resources in general, should be recognized as a technology option for the next generation of vehicles. Future research efforts should focus on enhancing powertrain models and conducting further vehicle testing. This entails developing adaptable powertrain models capable of accurately predicting pollutant emissions and fuel consumption for a range of carbon advanced fuels, as well as integrating ICE models and EATS components into a comprehensive powertrain simulation approach. Moreover, comprehensive testing campaigns with vehicle demonstrators should address the low-NOx capabilities of ICEs powered by renewable fuels in real driving conditions and at ambient temperatures below 0 degrees Celsius. Additionally, test campaigns featuring EU7 demonstrators using new fuels can provide valuable insights into the powertrain system and uncover potential challenges and opportunities, thereby contributing to a more holistic evaluation.

7 Acknowledgements

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Reference List

[EEA23] European Environment Agency (EEA): Greenhouse Gas Emissions by Source Sector., Eurostat Data Code: env_air_gge, https://ec.europa.eu/eurostat/databrowser/bookmark/1ffd5837-18ba-4e68-9634-1eaf2d6d4023?lang=de), last check: 31.05.2023.

[Sim24] Simon Völker, Niklas Groll, Marvin Bachmann, Leonard Müller, Marcel Neumann, Theodoros Kossioris, Paul Muthyala, Bastian Lehrheuer, Marius Hofmeister, Andreas Vorholt, Katharina Schmitz, Stefan Pischinger, Walter Leitner, and André Bardow: Towards carbon-neutral and clean combustion with hydroformylated Fischer-Tropsch fuels, (submitted)

[Sch20a] Schaub et al., Hybrid Powertrain Concepts for Light Commercial Vehicles, 29th Aachen Colloquium Sustainable Mobility 2020

[Sch20b] Schaub et al., Electrified efficiency – diesel hybrid powertrain concepts for light commercial vehicles, ATZ, Internationaler Motorenkongress 2020

[RegEU19] Regulation (EU) 2019/631 of the European Parliament and of the Council of 17 April 2019

[Neu18] Neumann, D., Pischinger, S., Zubel, M., Heuser, B., Thenert, K., Leitner, W., Schönen, M., Schaub, J., and Jörg, C. (2018). Power-to-Liquids - Kompensation variierender E-Fuel Zusammensetzungen mittels Digital Rate Shaping /Power-to-Liquids - Compensation of Varying E-Fuel Compositions via Digital Rate Shaping. In 39. Internationales Wiener Motorensymposium 26.-27. April 2018, B. Geringer and H.-P. Lenz, eds. (: VDI Verlag), pp. 230–258.