



Planetary boundaries analysis of Fischer-Tropsch Diesel for decarbonizing heavy-duty transport

Conference Paper**Author(s):**

[Charalambous, Margarita Athanasia](#) ; [Medrano-Garcia, Juan D.](#); [Guillén Gosálbez, Gonzalo](#) 

Publication date:

2022

Permanent link:

<https://doi.org/10.3929/ethz-b-000567756>

Rights / license:

[In Copyright - Non-Commercial Use Permitted](#)

Originally published in:

Computer Aided Chemical Engineering 49, <https://doi.org/10.1016/B978-0-323-85159-6.50328-6>

Funding acknowledgement:

180544 - NCCR Catalysis (phase I) (SNF)

Planetary boundaries analysis of Fischer-Tropsch Diesel for decarbonizing heavy-duty transport

Margarita A. Charalambous^a, Juan D. Medrano-Garcia^a, Gonzalo Guillén-Gosálbez^{a*}

^a*Institute for Chemical and Bioengineering, Department of Chemistry and Applied Biosciences, ETH Zürich, Vladimir-Prelog-Weg 1, 8093 Zürich, Switzerland*

**gonzalo.guillen.gosalbez@chem.ethz.ch*

Abstract

Here we evaluated Fischer Tropsch-diesel (FT-diesel) use in heavy-duty trucks based on various production pathways differing in the CO₂ and H₂ provenance. To better understand the global environmental implications of fuelling heavy-duty trucks (HD trucks) with FT-diesel, we quantified environmental impacts over the entire life cycle using seven Planetary Boundaries (PBs) regulating the Earth's resilience. Our environmental assessment follows a well-to-wheel scope with the functional unit based on the global annual freight demand. The baseline scenario corresponds to the conventional fossil fuel. Our results show that the fossil fuel alternative is unsustainable as it transgresses the climate change PBs. Using FT-diesel based on captured CO₂ could help operate within the safe operating space but it could induce critical burden-shifting if the CO₂ and H₂ sources are not adequately selected.

Keywords: Energy, Food and Environmental Systems

1. Introduction

In recent years, liquid fuels based on renewable carbon that can substitute conventional ones with minimal changes to current infrastructure have attracted increasing interest. Notably, fossil diesel can be replaced with "drop-in" fuels with similar or better characteristics. FT-diesel is a promising alternative to fossil diesel due to the high cetane number and improved properties with the potential to optimize combustion efficiency and decrease emissions.

So far, studies related to FT-diesel have focused mainly on the production process based on biomass as a raw material (Martín and Grossmann 2011), and very few on the CO₂-based production process (Al-Yaeshi et al. 2019). Environmental assessments of FT-diesel often quantify impacts based on conventional life cycle assessment (LCA) metrics (Holmgren and Hagberg 2009; Wernet et al. 2016), which are hard to interpret due to the absence of thresholds that can classify the studied systems as environmentally unsustainable. Hence, the absolute environmental sustainability implications of this fuel remain unclear.

Here we evaluated FT-diesel use in HD trucks based on various production pathways differing in the provenance of the raw material using seven PBs. The PBs concepts developed initially by Rockström et al., 2009, provides a framework to carry out absolute environmental sustainability assessments considering the Earth's carrying capacity. The framework considers 11 control variables linked to nine Earth's biophysical subsystems or processes. These include climate change, stratospheric ozone depletion, ocean acidification, biogeochemical flows of nitrogen and phosphorus, land system change,

freshwater use, biosphere integrity, atmosphere aerosol loading, and introduction of novel entities. All the PBs jointly establish the so-called safe operating space (SOS) for humanity. Consequently, for a scenario to be regarded as sustainable, none of the planetary boundaries should be transgressed. In essence, referring the LCA results to the safe operating space (SOS) delimited by these environmental guardrails facilitates the interpretation phase, particularly when evaluating systems that can be potentially deployed at a large scale. Based on this concept, we conducted an absolute environmental assessment over the global annual freight demand (33 trillion tkm), covering eight FT-diesel HD truck scenarios while benchmarking them against the fossil diesel HD truck counterpart –business as usual (BAU scenario)–. Hence, going well beyond standard LCAs, we analyze whether the FT-diesel trucks would help humanity operate safely within the PBs.

2. Methodology

2.1. Life cycle assessment and planetary boundaries

Following the general life cycle assessment (LCA) methodology, we carried out an environmental assessment based on the ISO 14040/44 framework using the SimaPro 9.0 software. The environmental assessment aims to assess the absolute sustainability of fuelling the global freight activities with FT-diesel from various sources. The functional unit corresponds to the global annual tkm demand for on-road HD truck activities, estimated by the International Energy Agency to be around $33 \cdot 10^{13}$ tkm.

For our analysis, we adopted a well-to-wheel scope using an attributional approach. The system boundaries cover all the upstream activities, from the production of H_2 and CO_2 , through the FT-diesel synthesis, to the fuel combustion in HD trucks. We estimated the life cycle inventory for FT-diesel by assuming that most of the emissions can be attributed to CO_2 and H_2 , as shown in Galán-Martín et al. (2021) for various bulk chemicals.

In order to construct the life cycle inventory, we first simulated the production of FT-diesel. Our calculations are based on the works of Shafer et al. (2019) for the FT-reactor, and Tomasek et al. (2020), for the wax hydrocracker. The Anderson-Shulz-Flory distribution (a) of choice for maximum diesel production is 0.88, and H_2/CO equals 2, based on which we calculated the product distribution of the FT-reactor. To calculate the total CO_2 and H_2 needed for the process, we assume that all the CO is converted into C_1 - C_{22} in the FT-reactor. Hydrocracking of the waxes was modelled according to Tomasek et al. (2020). The total production of diesel, gasoline, kerosene, and C_1 - C_4 , coming from the FT-reactor and the wax hydrocracker are summed in order to get the final products. Furthermore, the light ends are combusted to produce CO_2 , which is then recycled to the water-gas shift reactor (WGSR). Since gasoline and kerosene are co-produced, our LCA considers a system expansion approach with avoided burdens. The final inputs of the FT-diesel life cycle inventory are presented in Table 1.

Table 1: Life cycle inventory for the production of 1 kg FT-Diesel from CO_2 and H_2

FT-diesel	1	kg
Avoided products		
Gasoline	0.89	kg
Kerosene	0.72	kg
Inputs		
H_2	0.29	kg
CO_2	1.42	kg

The foreground system, i.e., truck and road constructions, etc., is based on the "Lorry 16-32 metric ton, EURO6" of the Ecoinvent v3.5 database. In essence, we consider the LCI for the BAU scenario, replacing the fossil diesel's inventory with that of FT-diesel, and adjusting the direct emissions based on Schemme et al. (2017). The scenarios differ in the origin of the educts (Figure 1). For this study, CO₂ is captured either from point sources at coal power plants, or directly from air (Coal and DAC). H₂ is produced through an electrolytic or thermochemical route. Polymeric water electrolysis is considered as the electrolytic route, powered by different energy sources, i.e., onshore wind, nuclear, and bioenergy with CCS (BECCS). Furthermore, for the thermochemical route, the conversion of biomass to hydrogen with carbon capture and storage (BTH CCS) is considered.

Data for the production of electrolytic H₂ were taken from Bareiß et al. (2019), considering for wind power a capacity factor of 0.34, respectively. For the different electricity sources, we used data from Ecoinvent v1.03, except for the BECCS scenario, based on Oreggioni et al. (2017). For the thermochemical route, the inventory was retrieved from Susmozas et al. (2016). Concerning the capture of CO₂, the Coal scenario is based on Iribarren, Petrakopoulou, and Dufour (2013), and the DAC scenario on Keith et al. (2018).

The life cycle impact assessment (LCIA) quantifies the absolute environmental sustainability level of FT-diesel by converting the LCI elementary flows into impacts on the control variables of seven PBs. Consequently, for a scenario to be regarded as sustainable, none of the planetary boundaries should be transgressed. Our study follows the characterization factors proposed by Ryberg et al. (2018) to quantify the impact on six PBs, together with the ones introduced by Galán-Martín et al. (2021) to evaluate the impact on biosphere integrity.

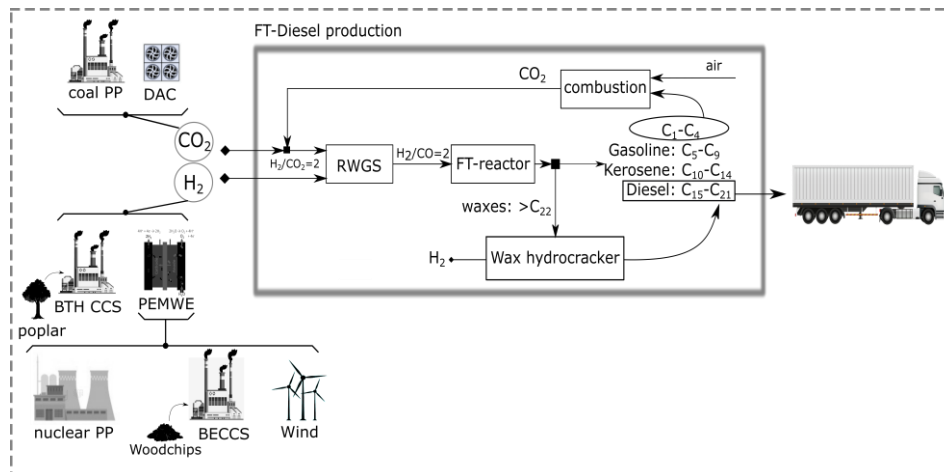


Figure 1: System boundaries of the different scenarios. From the production of CO₂ and H₂ from different sources to the production of FT-Diesel, and lastly, the end-use in HD trucks.

3. Results

3.1. Relative impact to the Safe Operating Space

Figure 2 shows that the current BAU scenario is unsustainable due to the transgressions of the climate change PB (CO₂, EI). Overall, all the FT-diesel scenarios have the potential to decrease the impacts of the BAU scenario. However, only two are sustainable, namely those based on DAC with electrolytic H₂ from nuclear, and H₂ from Biomass with CCS. These scenarios operate within the SOS for all the PBs. On the CO₂ boundary (75%, -140%, respectively), 1% and 2% in nitrogen flows (N-flows), and 7% and 25% in biosphere integrity (BII). All the remaining scenarios fail to be sustainable because they lead to burden-shifting to the N-flows and BII. Focusing on the scenarios with electrolysis routes powered with wind and nuclear electricity (DAC + Wind, DAC + Nuclear, coal + Wind, coal + Nuclear), undoubtedly, DAC scenarios would perform better than those relying on coal. The CO₂ coming from fossil resources was modelled as a positive emissions entry in contrast to the DAC scenario, where CO₂ is coming from the air, and hence is modeled as a negative emissions entry. Ultimately, these scenarios represent an interim solution as fossil fuels should be ultimately phased out. Scenarios that make use of CCS and biomass (DAC + BTH CCS, DAC + BECCS, coal + BTH CCS, coal + BECCS) show a great potential in the GHG-related PBs (CO₂, EI, OA), but lead to burden-shifting due to biomass growth. Notably, the N-flows are affected by the fertilisers, and the BII category by the use of land, e.g., DAC + BECCS and coal + BECCS take 30% of the SOS in the N flows.

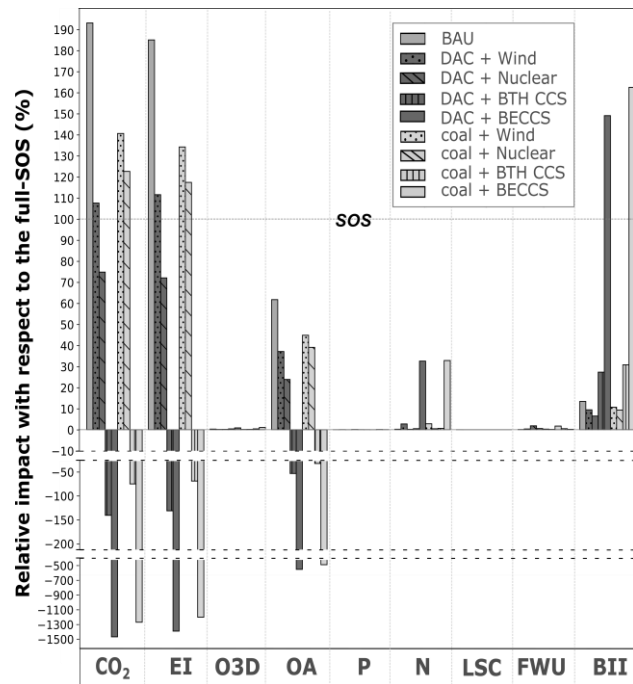


Figure 2: Relative impact in percentage of the safe operating space (SOS). The abbreviations of the PBs are: CO₂ (Climate change CO₂ concentration), EI (Energy imbalance), O3D (Stratospheric ozone depletion), P (Phosphorus flows), N (Nitrogen flows), LSC (Land system change), FWU (Fresh water use), BII (Biosphere integrity).

3.2. Impact breakdown

The breakdown of impacts in Figure 3 (upper) shows that most carbon-positive impacts come from the combustion emissions, i.e., 45%-85% of the total positive contributions in all the scenarios. Carbon negative impacts come from the biomass based scenarios with CCS (BTH CCS, BECCS), and are linked to the H₂ production. Electrolysis powered with BECCS has the most negative impacts due to the carbon-negative nature of the electricity generated, which requires large amounts of biomass. Furthermore, H₂ from nuclear performs 1.2-fold better in the CO₂ PB compared to H₂ from Wind. Regarding the CO₂ capture technologies, DAC is the only technology that can provide negative impacts since CO₂ is modelled as a negative emission entry. With regard to the biosphere integrity (BII), Figure 3 (lower) shows that the biggest impacts come BTH CCS and BECCS, with the latter being the worst. These high impacts are linked to the extensive land use for biomass growth. All the other scenarios perform better comparing to the BAU, however, it is important to mention that 65% of the carbon positive impacts are coming from the combustion emissions and 25% from the construction of roads.

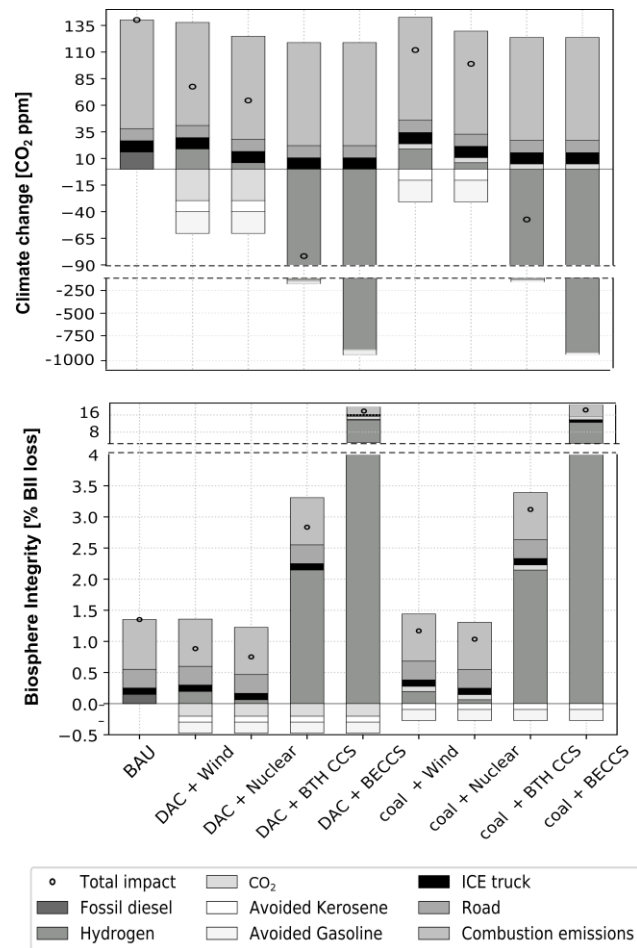


Figure 3: Breakdown of impacts in the CO₂ boundary (upper), nitrogen flows (middle), and biosphere integrity (lower).

4. Conclusions

Using CO₂-based fuels has attracted increasing attention, yet their broad sustainability implications remain unclear. Here we assessed the absolute environmental sustainability of FT-diesel from renewable carbon as an alternative fuel for HD trucks using seven planetary boundaries (PBs). We found that the current fossil-based fuel alternative transgresses the climate change-related PBs, while renewable-carbon fuels could help operate within these ecological limits. However, burden-shifting to BII and N-flows may occur. This collateral damage would be more critical in the biomass-related scenarios, which remove large amounts of CO₂ but need land and fertilisers for biomass growth. Hence, the CO₂ and H₂ sources for producing these fuels should be selected carefully to mitigate climate change without exacerbating the damage in other critical Earth-system processes, thereby preserving the planet's stability.

Acknowledgements: This work was created as part of the NCCR Catalysis, a National Centre of Competence in Research funded by the Swiss National Science Foundation.

References

- Al-Yaeshi, Ali Attiq, A. AlNouss, Gordon McKay, and T. Al-Ansari, 2019, "A model based analysis in applying Anderson-Schulz-Flory (ASF) equation with CO₂ utilisation on the Fischer Tropsch gas-to-liquid process.", *Computer Aided Chemical Engineering*, 46, 397–402.
- Bareiß, Kay, Cristina de la Rua, Maximilian Möckl, and Thomas Hamacher, 2019, "Life cycle assessment of hydrogen from proton exchange membrane water electrolysis in future energy systems.", *Applied Energy*, 237, 862-72.
- Galán-Martín, Ángel et al., 2021, "Sustainability footprints of a renewable carbon transition for the petrochemical sector within planetary boundaries." *One Earth*, 4, 565–83.
- Goedkoop, Mark et al., 2016, "Introduction to LCA with SimaPro Colophon." "Introduction to LCA with SimaPro."
- Holmgren, Kristina, and Linus Hagberg, 2009, "Life cycle assessment of climate impact of Fischer-Tropsch diesel based on peat and biomass."
- Iribarren, Diego, Fontina Petrakopoulou, and Javier Dufour., 2013, "Environmental and thermodynamic evaluation of CO₂ capture, transport and storage with and without enhanced resource recovery." *Energy*, 50, 477–85.
- Keith, David W., Geoffrey Holmes, David St. Angelo, and Kenton Heidel, 2018, "A process for capturing CO₂ from the atmosphere.", *Joule*, 2, 1573–94.
- Li, Pengcheng, Zhihong Yuan, and Mario R. Eden, 2016, "A comparative study of Fischer-Tropsch synthesis for liquid transportation fuels production from biomass.", *Computer Aided Chemical Engineering*, 38, 2025–30.
- Martín, Mariano, and Ignacio E. Grossmann. 2011. "Process optimization of FT-diesel production from lignocellulosic switchgrass." *Industrial and Engineering Chemistry Research* 50(23): 13485–99.
- Oreggioni, Gabriel D. et al. 2017. "Environmental assessment of biomass gasification combined heat and power plants with absorptive and adsorptive carbon capture units in Norway." *International Journal of Greenhouse Gas Control*, 57, 162–72.
- Rockström, J. et al. 2009. "A Safe operation space for humanity." *Nature*, 46, 472–75.
- Schemme, Steffen, Remzi Can Samsun, Ralf Peters, and Detlef Stolten. 2017. "Power-to-Fuel as a key to sustainable transport systems – An analysis of diesel fuels produced from CO₂ and renewable electricity." *Fuel*, 205, 198–221.
- Shafer, Wilson D. et al. 2019. "Fischer-Tropsch: Product selectivity-the fingerprint of synthetic fuels." *Catalysts*.
- Susmozas, Ana et al., 2016, "Life-Cycle performance of hydrogen production via indirect biomass gasification with CO₂ Capture." *International Journal of Hydrogen Energy*, 41, 19484–91.
- Szabina Tomasek, Ferenc Lonyi, Jozsef Valyon, Anett Wollmann, Jenő Hancsok., "Hydrocracking of Fischer-Tropsch paraffin mixtures over strong acid bifunctional catalysts to engine Fuels."