

Environmental Benefits of Combined Electro-Thermo-Chemical Technology over Battery-Electric Powertrains

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Electric vehicles are being promoted worldwide in an attempt to mitigate greenhouse gas emissions and improve air-quality in cities. Yet, alternative propulsion systems could allow meeting climate change and air-quality policy goals while not raising other environmental impacts. This study offers a glimpse into the wide range of mobility solutions aside from traditional battery-electric vehicles (BEVs). We perform a comparative life-cycle assessment of a BEV with a vehicle comprised of a novel combined electro-thermo-chemical (CETC) propulsion technology composed of a fuel-cell (FC), an internal-combustion engine (ICE) and thermochemical recuperation (TCR) of waste heat. A comprehensive comparison was conducted across multiple categories of environmental impacts for the two technologies from the stage of manufacturing, through vehicle use and vehicle end-of-life. Our findings demonstrate that a vehicle comprised of the new CETC technology outperforms the BEV for the majority of environmental impacts, including climate-change, air-pollution and other human-health and ecological impact categories.

1. Introduction

Due to the significant contribution of the transportation sector to global climate change, the future of transportation technologies is part of the ongoing climate change discourse. Accordingly, reduction in greenhouse gas emissions and mitigation of air pollution arising from traditional fossil fuel-based transportation are a central focus of public concern and discussion. The global ecological impacts of the propulsion technologies under consideration must be addressed, as their manufacturing and subsequent energy production and transformation can have significant negative ecological impacts such as terrestrial acidification and water eutrophication.

Life cycle assessment (LCA) is a widely accepted tool that enables quantifying and evaluating the emissions and environmental impacts of a product system over its entire life cycle. This includes all life stages starting from raw materials extraction, manufacturing, use, and end-of-life management. LCA aids in identifying the hotspots

in a system or field and subsequently assists in guiding both early-stage research and policy-making.

Multiple studies have shown that the non-use phases in a vehicle's lifetime, regardless of the propulsion system, are significant contributors to lifetime total emissions and environmental impacts, requiring their consideration while evaluating the ecologic impact of any system [1-3].

Here, we use LCA to comprehensively evaluate the integration of the combined electro-thermo-chemical (CETC) propulsion technology in vehicles as a more environmentally preferable alternative to battery electrical vehicles (BEVs). This work provides a different view compared to prior LCA studies, which mostly compared BEVs and internal combustion engine (ICE) vehicles or fuel-cell (FC) driven vehicles [4-16].

1.1 The Novel CETC Powertrain

The CETC technology is well suited for use in transportation (especially maritime and heavy-duty road vehicles) and consists of a fuel cell and the well-known internal combustion engine, both utilizing thermo-chemical recuperation of the waste heat for onboard hydrogen production. FCs produce electrical work by electrochemical reaction between a fuel and oxygen sourced from ambient air. In this reaction heat is produced also due to irreversible processes. The suggested CETC powertrain is fed with methanol as the primary fuel source for both the ICE and FC. Methanol is an excellent electro-fuel that can be renewably produced using captured CO₂ [17]. In the considered CETC powertrain, methanol is reformed to a hydrogen-rich reformat. The reforming process is accomplished by recuperating waste heat produced in both the ICE and FC in a TCR process, consequently enabling an increased efficiency of the system [18]. A schematic outline of the CETC powertrain is presented in Fig. 1.

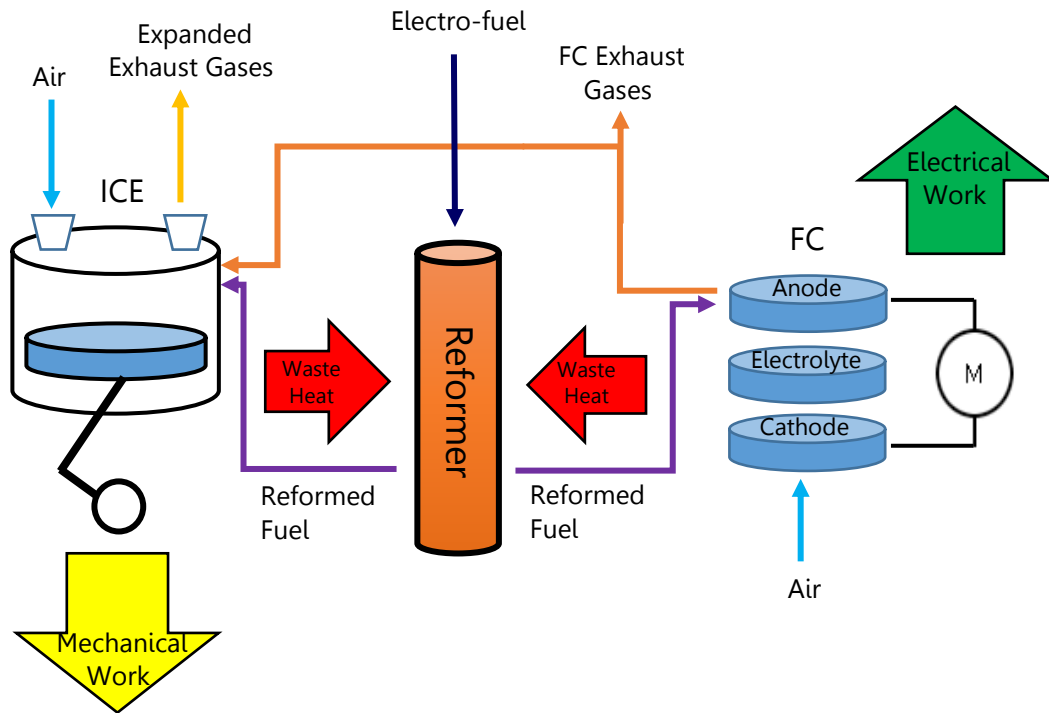


Figure 1 – A summarized scheme of the CETC powertrain. Fuel enters the reformer, which is activated by heat recovered from FC and ICE. The reformed fuel (reformate) is supplied to the FC and ICE.

Hybrid FC-ICE powertrains have been studied since the 1990s [19, 20]. In our previous studies, we examined the power and efficiency relation of these powertrains [21-23] and proposed the new CETC cycle with TCR. The FC type in the suggested powertrain was selected to be a solid-oxide FC (SOFC). SOFCs can operate with fuels other than pure hydrogen, and their high operating temperature favors the TCR process. Due to its high-density energy source, the proposed CETC powertrain with TCR is lighter than the battery-electric alternative. Fig. 2 clearly demonstrates that the CETC technology offers a power increase at the same efficiency over sole FC operation [20]. The significant power gain is maintained up to high efficiencies of 70% and beyond.

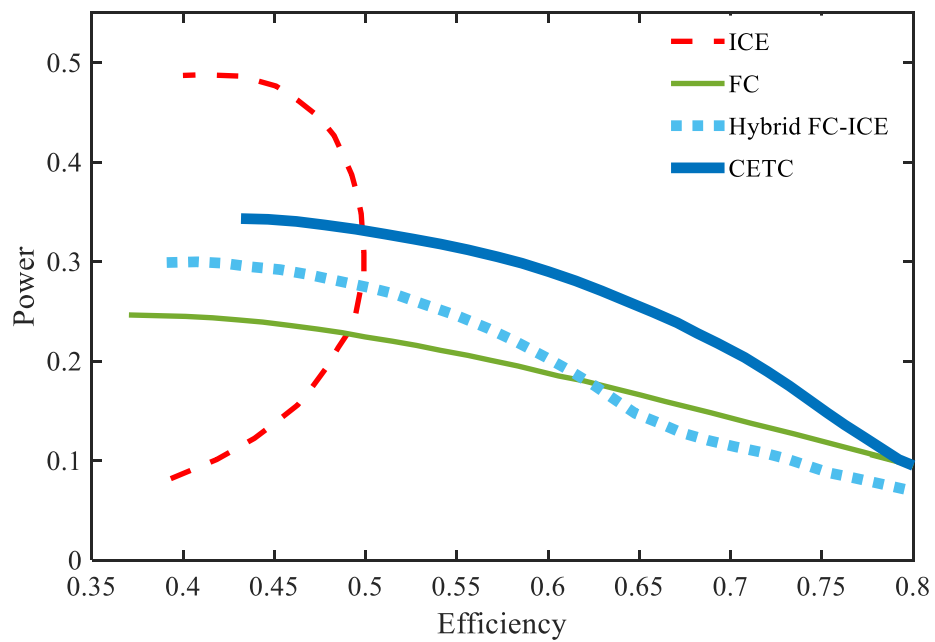


Figure 2 – Power-efficiency relationship of various propulsion technologies.

Moreover, the CETC powertrain enables a flexible and dynamic operation that utilizes the benefits of both FC and ICE. For example, at low-power loads the highly efficient FC can be the sole supplier of power, while for the short time intervals where high power is demanded, the ICE is utilized. This combination allows a high system efficiency and vehicle weight reduction, resulting in a decrease in overall energy use. Additionally, the implementation of the CETC powertrain is convenient as liquid fueling is quick, familiar and supported by a widespread and accessible infrastructure.

The main research question examined in this study is whether the proposed CETC powertrain is superior compared to the common battery-electric powertrain. In our view, this question should be divided into two parts. The first is assessing environmental concerns like climate change, air pollution and other ecologic burdens. This issue is discussed in the following sections of this article using LCA of the suggested CETC propulsion in comparison to a BEV. The second matter to be considered is the feasibility of commercializing CETC technology, addressing whether technological gaps can be bridged within a reasonable timeframe. A discussion of the second question appears towards the end of this article.

2. Materials and Methods

2.1 Goal and Scope

To comprehensively evaluate the environmental impacts of the novel CETC technology with the conventional battery-electric powertrain, an LCA approach based on the ISO standards 14040/14044 [24, 25] was chosen. The LCA is divided into two sub-cycles: the fuel cycle and the vehicle cycle (Fig. 3).

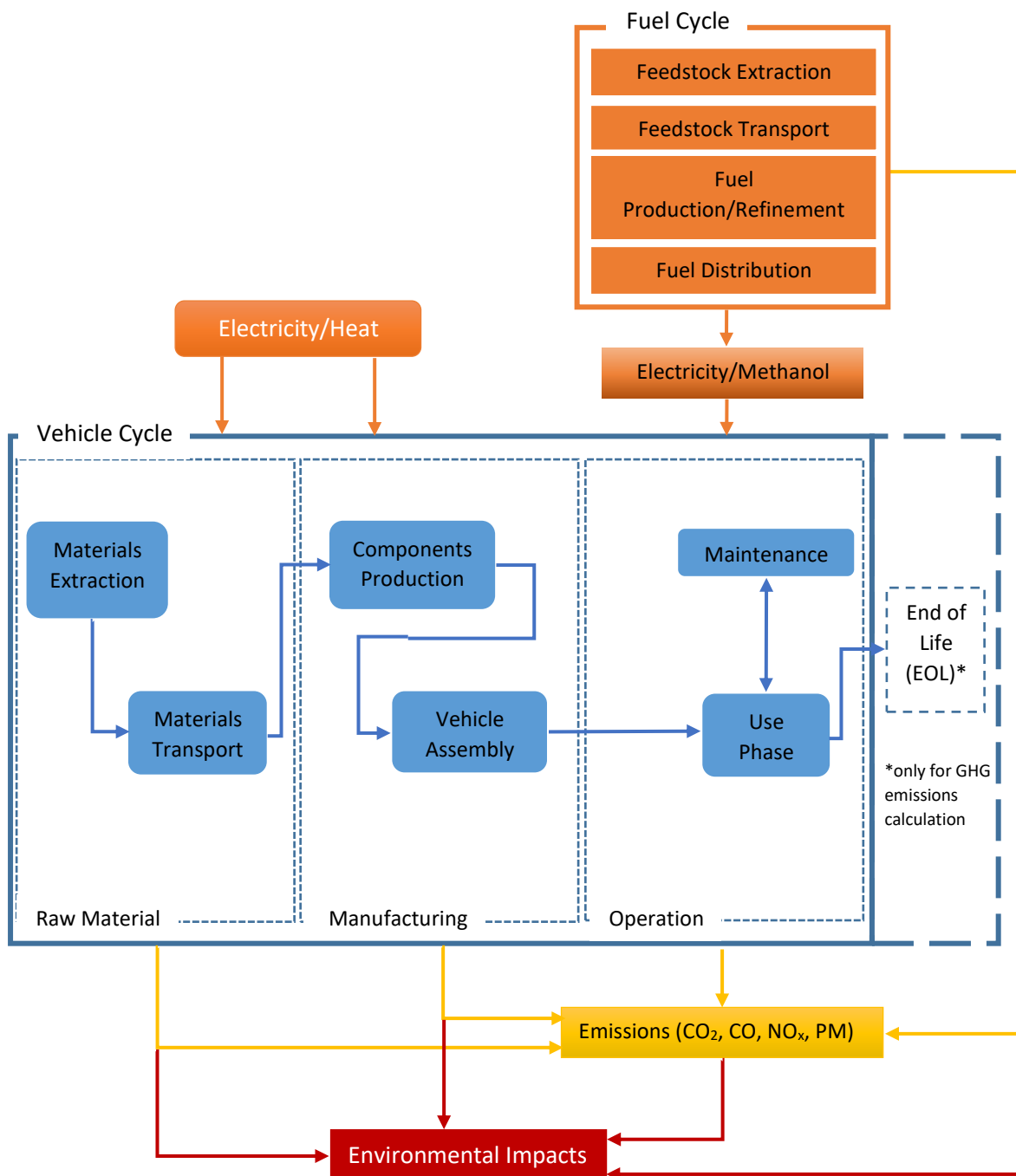


Figure 3 – System boundaries for the LCA, and details of the two sub-cycles: fuel cycle and vehicle cycle.

The fuel cycle includes the extraction of the fuel feedstock, transportation of the feedstock, fuel production from the feedstock and distribution of the fuel to the fueling stations (defined as well-to-pump (WTP)).

The vehicle cycle boundaries (cradle-to-grave (CTG)) contain the following processes: material extraction and transportation, vehicle component production, vehicle assembly, vehicle operation that includes the use phase and the vehicle maintenance, and vehicle end-of-life (EOL), which addresses the recycling and disposal stages. The environmental impacts examined are contributed by all the processes defined in the LCA boundaries except for the vehicle EOL stage, which only contributes to GHG emissions and not to the other environmental impacts. The latter is due to lack of reliable data referring to the full environmental impact of the disposal and recycling stages.

It is important to note that this LCA study excludes the impacts of building and maintenance of the infrastructures required throughout a vehicle's lifecycle. For example, the impact of building the copper demanding charging stations for the BEVs is not calculated in the considered LCA. This exclusion is highly favorable towards the BEV lifecycle because the novel CETC technology does not necessitate new infrastructure.

2.2 Characterization of the Selected Case Study

The case study selected for a comparative analysis is a pick-up truck (PUT), which functions as a midpoint vehicle type between the passenger cars and heavy-duty trucks. While the results discussed in this study apply to PUTs, the conclusions may be applicable to other vehicle classes, especially heavier vehicles and even marine applications. The latter applies, as ICEs tend to operate more efficiently at larger scales, while FC and battery performance is indifferent to scale.

The lifetime of the vehicle in the operation phase (defined as pump-to-wheels - PTW) is determined by its total mileage, which in the selected case study is 300,000 km. Additionally, the PUTs are composed of conventional materials rather than advanced lightweight materials.

The proposed primary fuel for the CETC technology is methanol. Two methanol-production scenarios were examined. First, the standard US methanol made from NG with US electricity mix. Second scenario: 90% replacement of the standard methanol with electro-fuel, using captured CO₂ and renewable energy for production. Similarly, two fuel cycles were examined for BEV electricity production. First, US

electricity generation (US electricity mix), and second, replacement of 90% with renewably produced electricity.

The miles per gallon equivalent (MPGe) of both vehicles was weighted at 43% city operation and 57% highway operation, consistent with the U.S. Environmental Protection Agency (EPA) real-world fuel economy calculation method [26].

The weight of the CETC powertrain (with methanol-steam-reforming based TCR) was calculated using the power-efficiency relation displayed in Fig. 2 with maximum power output of 220[kW], meeting the power output of a modern PUT.

The contribution of the FC and the ICE to total power supply and total efficiency varies according to the PUT's load (Fig. 2). The PUT's operation phase was tested using the EPA's fuel economy calculation methods using both highway and urban driving cycles - the Highway Fuel Economy test (HWFET) and the Federal Test Procedure (FTP) respectively.

The BEV PUT parameters were selected from the GREET 2022 database for a vehicle traveling up to 500 mi. Powertrain properties of the FC, ICE and BEV are summarized in Table 1.

Table 1 – Specifications of the different powertrains.

FC Specifications		ICE Specifications		BEV500 Specifications	
Fuel stack size [kg]	337	Max IMEP (bar)	6	Mileage [km]	707.7
Fuel Cell Type	SOFC	Max Speed (rpm)	6000	Battery Type	Li-ion
Operating Temperature	650-850°C	Maximum Power Demand (kW)	84.95	Battery Size [kWh]	247.8
Heat-up Time [sec]	180	Number of Cylinders	6	Electric Powertrain Efficiency	90%
Maximum Power Demand (kW)	135.6	Max Power per Cylinder (kW)	14.16	Charger Efficiency	85%
Weight-to-Power Ratio [kg/kW]	1.275	Cylinder Displacement (cm³)	471.9	Fuel Economy [MPGe]	59.8
		Total Displacement (cm³)	2831.67	Battery Weight [kg]	1170
Reformer weight [kg]	8	Fuel Supply Method	Direct injection		
Total CETC Driven Vehicle Weight [kg]	2199	Ignition type	Spark ignition	Total BEV Weight [kg]	2974

2.3 Summary of methods used for each stage.

The simulations were performed using three tools: 1. GREET 2022 (Greenhouse gases, Regulated Emissions, and Energy use in Transportation) full life-cycle assessment model from the U.S. Argonne National Laboratory [27, 28], 2. SimaPro with ecoinvent [29] 3.8 version database, and 3. A MATLAB based dynamic vehicle model used for fuel economy and emissions calculation of the vehicle powered with the CETC powertrain. A summary of the tools use over the different phases and vehicles is shown in Table 2.

Table 2 - Summary of tools used for each phase and vehicle.

	<u>BEV</u>			<u>CETC Vehicle</u>		
	GHG	Air Pollution	Ecological Impacts	GHG	Air Pollution	Ecological Impacts
Feedstock & Fuel	GREET1 & GREET2	GREET1 & GREET2	GREET1 & GREET2 & SimaPro & Ecoinvent 3.8	GREET1	GREET1	GREET1 & SimaPro & Ecoinvent 3.8
Production	GREET2	GREET2	GREET2 & SimaPro & Ecoinvent 3.8	GREET2 & SimaPro & Ecoinvent 3.8	GREET2 & SimaPro & Ecoinvent 3.8	GREET2 & SimaPro & Ecoinvent 3.8
Operation	GREET2	GREET2	GREET2 & SimaPro & Ecoinvent 3.8	Self-Developed MATLAB model	Self-Developed MATLAB model	Self-Developed MATLAB program & SimaPro & Ecoinvent 3.8
Disposal	GREET2	N/A	N/A	GREET2	N/A	N/A

2.4 Life cycle inventory (LCI)

Several data sources were used to build the LCI. For GHG emission and air pollution GREET 2022 was used to gather the metrics for the fuel cycle and vehicle cycle for both vehicles. The BEV was defined as a PUT made from conventional materials and battery capacity capable of 500 miles between charges (EV500). The CETC vehicle material composition, processes and weights is based on the GREET 2022 database, except for the SOFC and the reformer. The data for the SOFC was gathered from the work of

Teixeira Taboada [30] and the data for the reformer is based on the reformer of Sall et al. [31, 32] using Belcastro [33] data on the materials and production processes. SOFC and reformer data from the studies above were used for the whole LCA including for the assessment of the ecological impacts. The components weight of both vehicles is summarized in Table 3.

Table 3 - Component weight and vehicle total weight comparison

Component	BEV [kg]	CETC Vehicle [kg]
Powertrain System (including BOP)	27.7	452
Transmission System	68.9	68.9
Chassis (w/o battery)	638	630
Traction Motor	189	82.4
Electronic Controller	104	72.4
Fuel Storage System	-	26.3
Body: including BIW, interior, exterior, and glass	740	740
Battery	1170	24.2
Fluids (excluding fuel)	33.9	38.4
Fuel	-	62.3
Curb Weight	2974	2199
<u>Total Weight</u> <u>(with cargo and passengers)</u>	<u>3110</u>	<u>2335</u>

Vehicle component replacements during lifetime are considered as well, detailed in the Table 4.

Table 4 – component replacement

Component replacement over lifetime	BEV	CETC Vehicle
Tires	4	4

Lead acid Battery	-	2
Engine oil	-	44
Brake fluid	4	4
Transmission fluid	1	1
Powertrain coolant	4	4
Windshield fluid	22	22

The fuel cycle is divided in GREET1 into two main sub-stages – feedstock stage and fuel stage. The feedstock stage includes the production, transport and storage of the fuel’s feedstock. The fuel stage includes the production, transport, distribution, and storage of fuel that will be consumed by vehicle. For BEVs, the fuel stage includes electricity production and transport. The energy use, emissions and environmental impacts of each fuel path were calculated using GREET1. Accordingly, for each system different fuel pathways that vary by feedstock source, fuel production method and electric generation mix were inspected. For BEVs these are mainly dependent on the electricity generation mix the BEV is reliant upon for electricity. Thus, the emissions are directly correlated to the electricity production grid mix, efficiency of production and transport, and the extent of reliance on renewable electricity generation methods. Comparable to the BEV and electricity production, the methanol fuel path used for the proposed CETC powertrain is analyzed considering production method, production efficiency, plant design and feedstock source – all affecting the system lifetime emissions and environmental impacts. Additionally, the means of transportation and distribution of the fuel contributing to the above are considered as well. Electricity production and distribution for BEV charging is based on the US electricity mix as defined by GREET 2022 (Table 5). The Methanol used by CETC vehicle is produced from North American NG as specified in GREET 2022.

Table 5 – US Electricity mix.

US Electricity Mix	
Residual oil	0.3%
Natural gas	36.5%

Coal	23.8%
Nuclear power	19.6%
Biomass	0.3%
Hydroelectric	6.5%
Geothermal	0.4%
Wind	9.4%
Solar PV	2.7%
Others	0.5%

As for ecological impacts, the material composition, processes and weights of the vehicle components obtained from GREET 2022 were adapted to the ecoinvent 3.8 database similar to the LCI of ref [13] and was calculated according to ReCiPe 2016 Midpoint (H) V1.07 / World (2010) H Method [34]. The ReCiPe midpoint hierarchical approach has been used to evaluate a wide variety of engineering systems including, water treatment and infrastructure [35], manufacturing [36] and multiple prospective renewable energy systems [37].

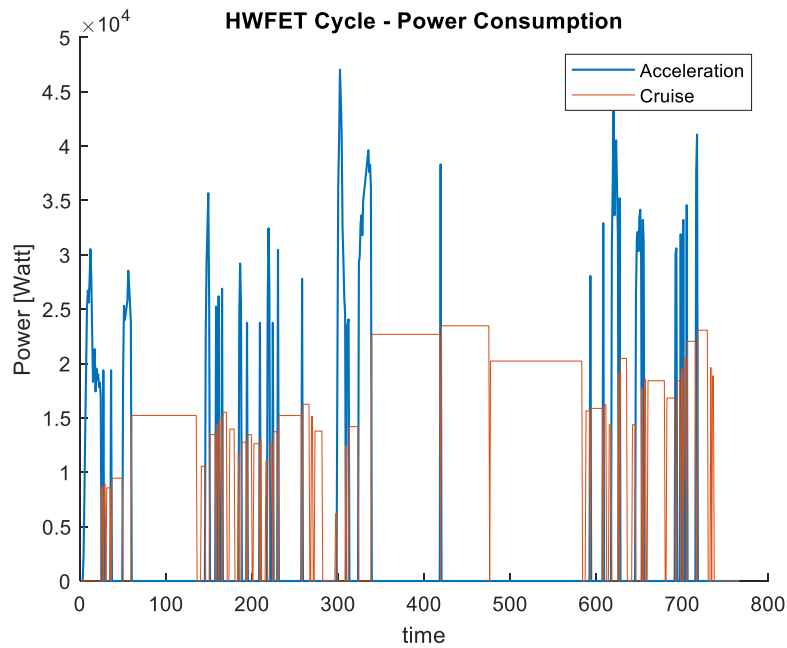
2.5 Emissions calculation of CETC operation phase

A MATLAB numeric model was developed and employed for the operation phase of the CETC vehicle. The output from the MATLAB model is pollutant emissions and the CETC-driven PUT fuel economy in both highway- and city-driving scenarios. The maximal power-to-weight ratio of the ICE is set to be twice as big as the maximal power-to-weight ratio of the FC. This is in accordance with modern ICE and FC technologies [38]. Accordingly, the weight ratio between the ICE and FC systems is 0.24 and 0.76 respectively. Thus, the weight of CETC powertrain and its components was found to be as outlined in Table 6.

Table 6 – Weight of CETC powertrain components

Powertrain Component	ICE	FC	Reformer	Total
Weight [kg]	106.59	337.55	8	452.14

The power supplied by each subsystem varies according to the PUT's load, thus making the contribution of the FC and the ICE to total power supply fluctuate, and with it the CETC powertrain efficiency. Based on Fig. 2, at maximum power output of 220[kW], the CETC powertrain was found operating at $\eta_{f,HV} = 43\%$, while operation at maximal efficiency of $\eta_{f,HV} = 70\%$ supplies 112[kW] of power. It was found that during both the FTP cycle and HWFET cycle, the CETC power demand is below the 112[kW] threshold, allowing for operation at maximum efficiency throughout both driving scenarios (Fig. 4). Accordingly, for all points in the dynamic MATLAB model, the CETC powertrain efficiency is assumed to be $\eta_{f,HV} = 70\%$ with a power supply delivered by the ICE and FC at a share of 32% and 68% respectively. The latter was calculated using the data of Fig. 2.



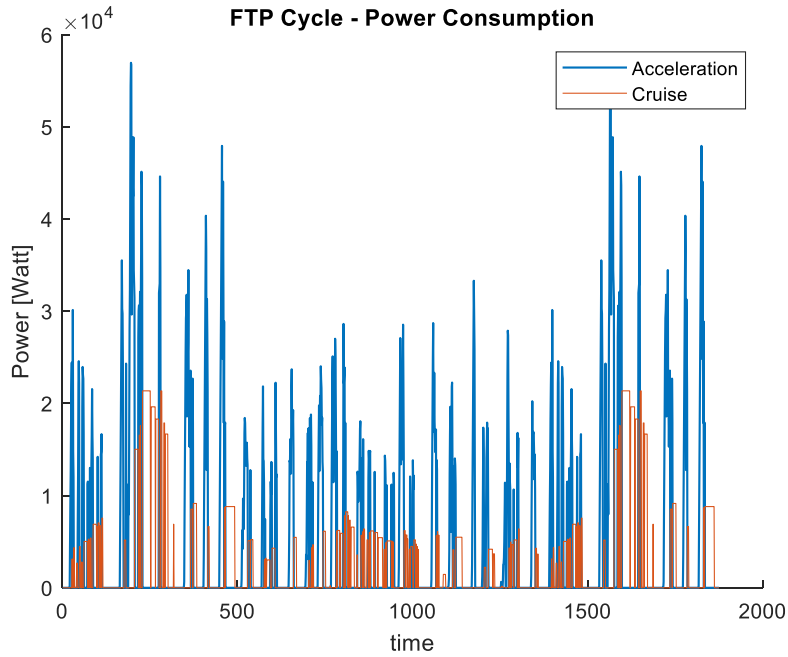


Figure 4 – Top: CETC vehicle power demand during HWFET cycle; **Bottom:** CETC vehicle power demand during FTP cycle

Over a vehicle's lifecycle, it rarely operates at maximum power, allowing the CETC powertrain to operate at the high end of its efficiency range. Furthermore, during city driving the FC can operate alone, allowing for the mitigation of the tailpipe pollutant emissions. This allows for the mitigation of pollutant emissions and the subsequent increased risk to human health caused by traffic and congestion in the city. Thus, similar to the BEV's operational stage, potential CO and NO_x emissions will be eliminated during urban operation. Accordingly, the FC efficiency was set to 65% in accordance with the efficiency of current SOFC technologies [38], consequently making the efficiency of the CETC powertrain in the city cycle $\eta_{f,FC} = 65\%$. The ICE specifications were selected as follows: The highest indicated mean effective pressure (imep) was set to be 6[bar] to comply with previous studies where the engine with TCR emissions were measured up to an imep of 6[bar] [39]. Additionally, the minimal imep of the ICE was set to be 2[bar], to prevent the air-fuel mixture from becoming too lean and performing low-pressure direct injections.

The vehicle Drag coefficient of the CETC PUT was selected to be equivalent to that of a 2019 Ram1500 light duty PUT – $C_d A = 1.21 [m^2]$. The frontal drag coefficient is calculated by multiplying the vehicle's frontal area $A [m^2]$ with its drag coefficient C_d

. Note that for both BEV and CETC PUTs the drag coefficient is equal, even though the BEV PUT is heavier, and thus might be larger. Therefore, the latter is a strict assumption for the CETC PUT calculation. The PUT's Rolling coefficient was selected to be a constant value of $C_R = 0.015$. Gradient resistance was neglected in this model as the EPA dynamometer test is performed at zero incline. The selected transmission efficiency of the CETC powertrain was set at 90%.

In previous studies where the ICE with TCR system was tested in the laboratory, the emission data was acquired with the ICE operating at 2700[rpm] [39]. Hence, this speed was selected for emission calculation in the model.

A Summary of vehicle parameters required for the MATLAB model is presented in Table 7.

Table 7 – CETC vehicle parameters.

Vehicle Parameters	
Vehicle Weight (with cargo and passengers) [kg]	2335
Frontal Drag coefficient [m²] ($C_D A$)	1.21
Rolling Coefficient	0.015
Transmission Efficiency	0.9
ICE Speed [rpm]	2700

The data provided by the EPA included velocity vs time dependence (detailed speed change over 1 second increments) for both FTP and HWFET cycles. The fundamental concept of the model required a division of the driving sequences into different operation modes. As defined in previous studies, vehicle driving can be divided into four operating modes – acceleration, cruising, deceleration, and idling [40, 41]. As shown earlier, each cycle is characterized by varying driving patterns. For example, during the HWFET test, the vehicle has zero idling time.

Each operation mode has a different power calculation equation which represents the PUT power demand. After defining the power requirement of the PUT throughout the driving cycle, the fuel consumption was calculated. This was done for both the FTP and HWFET cycles, allowing for the calculation of fuel economy during city and highway driving.

Cruising mode – was defined as either a non-zero speed unchanged from the previous second or an absolute speed change that was smaller than 0.2 [m/s] from that of the previous second.

$$P_{\text{Cruising}} = 1/\eta_T \left(\underbrace{C_R M_V \cdot g}_{\text{Rolling Resistance}} + \underbrace{\frac{1}{2} \rho_a C_D A_V v^2}_{\text{Aerodynamics Resistance}} \right) v$$

Acceleration mode – was defined for all accelerations greater than 0.2 [m/s²].

$$P_{\text{Acc}} = 1/\eta_T \left(M_V a + \underbrace{C_R M_V \cdot g}_{\text{Rolling Resistance}} + \underbrace{\frac{1}{2} \rho_a C_D A_V v^2}_{\text{Aerodynamics Resistance}} \right) v$$

Deceleration - was defined for all decelerations greater than 0.2 [m/s²]. As shown in [41], vehicle decelerating, or breaking does not result in energy expenditure and thus does not consume fuel. This is assuming the vehicle has a declaration fuel cut-off (DFCO) system that automatically cuts the fuel supply when coasting or braking in order to achieve better fuel efficiency and more effective engine braking.

$$P_{\text{Deceleration}} = 0$$

Idling – was defined for when the vehicle's speed is zero. This occurs only in the FTP cycle when only the FC is operating. As a result, the power use is defined by the minimal fuel consumption required for FC operating temperature conservation. This value was estimated to be 10% of the average fuel consumption during vehicle acceleration in the FTP cycle.

After calculating the required power during each cycle, the fuel economy was converted using the following equation:

$$\dot{m}_f = \frac{P}{\eta_f Q_{HV}} \rightarrow MPGe_{\text{City}}^{2\text{cy}} = 64.52 \quad ; \quad MPGe_{\text{HW}}^{2\text{cy}} = 76.13$$

As detailed earlier, the CETC powertrain efficiency η_f differs in each driving cycle.

During highway driving the baseline value was chosen to be $\eta_f = 70\%$ while both ICE and FC operate, However, while in city driving, the baseline value was selected to be $\eta_f = 65\%$, equivalent to the SOFC efficiency as only the FC is operating.

After calculating the fuel economy in the city and highway cycles in the MATLAB numeric model, it was required to correct them according to EPA's 5-cycle methodology. This included the use of the following equations resulting in a corrected fuel economy label:

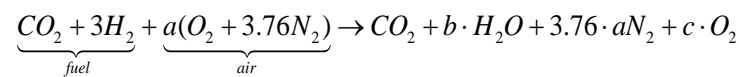
5 Cycle Method:

$$MPGe_{City}^{5cy} = \frac{1}{\left(0.004091 + \frac{1.1601}{MPGe_{City}^{2cy}}\right)} = 43.84 \quad ; \quad MPGe_{HW}^{5cy} = \frac{1}{\left(0.003191 + \frac{1.2945}{MPGe_{HW}^{2cy}}\right)} = 49.52$$

$$\rightarrow MPGe_{label} = MPGe_{City}^{5cy} \cdot 0.43\% + MPGe_{HW}^{5cy} \cdot 0.57\% = 47.08$$

The CETC vehicle's Fuel economy was found to be 47.1 MPGe. This is compared to that of the electric BEV500 in GREET1 which was calculated as 59.8 MPGe.

After finding the CETC vehicle's fuel consumption, the CO₂ emissions can be directly and easily calculated. The leading chemical reaction equation is as follows:



For the CETC vehicle emissions in the operation stage, previous laboratory experiments and results were used [39]. The data included CO, NO_x and PM10 emissions during a range of varying engine imep, allowing for the derivation of emission-imep correlation equations. The calculated vehicle power use throughout the vehicle cycle was then correlated to engine imep, allowing for the integration of the laboratory data in the numeric model.

3. Results and Discussion

3.1 Environmental aspects

First, GHG emissions were examined in two scenarios, one at a national level assuming the US electricity production grid mix, and second, a future-anticipated renewable energy mix, as was detailed in the previous sections of the article. The results are presented in Fig. 5a. GHG emissions are displayed in grams of CO₂ equivalent per km traveled (gr/km) for each technology.

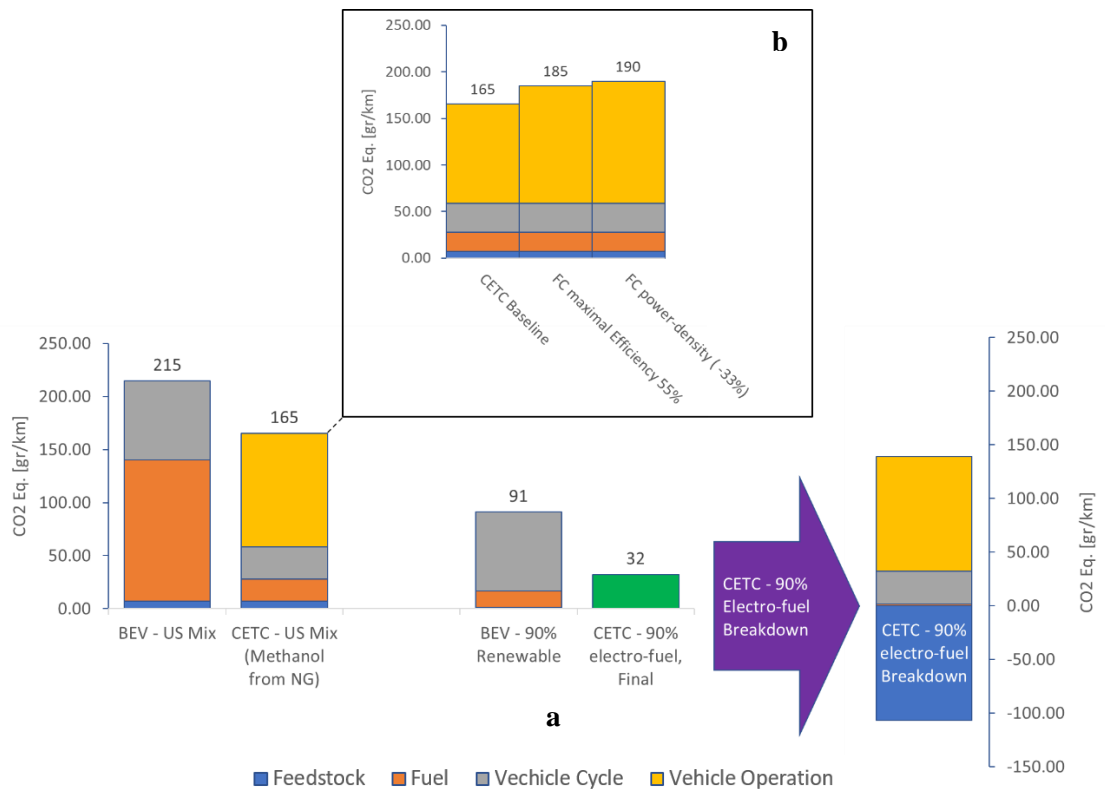


Figure 5 – Vehicle's full life cycle GHG emission. **a** - comparison between BEV and CETC vehicles for two scenarios: US mix (left) and 90% renewable energy (right). **b** - sensitivity analysis of the CETC GHG emission.

While the BEV powertrain efficiency is higher than the CETC powertrain efficiency (~90% compared to 65%-70%, respectively), the overall energy demand and the subsequent CO_{2,Eq} emissions of the CETC vehicle are **lower**. This is due to three main reasons: 1) the CETC vehicle is lighter than the BEV by more than 20%; 2) the overall efficiency of the BEV including electricity production, transport and charging reaches a similar efficiency of the CETC vehicle including methanol production (~41%); and 3) the energy demand required in the BEV production phase is considerably higher than that of the CETC powertrain-based PUT. Indeed, it was found that energy demand for the BEV vehicle cycle is higher by almost 250% compared to the CETC vehicle cycle. The latter is mainly due to the complexity of battery materials extraction and disposal/recycling [42]. Notably, the production of Li-Ion batteries accounts for over 70% of the total energy demand of the BEV production phase.

Still, there is one parameter - the overall efficiency of the CETC powertrain - that relies mostly on simulation results and was not proven sufficiently by experimental studies [21]. This parameter varies with power demand and depends strongly on the FC performance. Therefore, a sensitivity analysis of the FC power-efficiency

dependency and FC maximal efficiency was performed. It is assumed that the performance data used for the ICE is accurate. In Fig. 5b the GHG emissions are presented for the US energy production mix, with FC maximal efficiency reduction to $\eta_{max,FC} = 55\%$ (instead of $\eta_{max,FC} = 65\%$) and power-density reduction by 33% (which result in 50% increase of FC size). It can be seen from Fig. 5b that even for lower power-densities and lower FC efficiencies the CETC driven-vehicle outperforms the BEV in terms of GHG emissions.

Although the GHG emission results are an important outcome of the LCA comparison showing the potential of the compared powertrains regarding climate change, other environmental impacts should be analyzed for a complete picture. Fig. 6 shows the results of air quality impacts, including carbon-monoxide (CO), NO_x and particulate matter (PM) pollutants. It must be emphasized that both BEV and CETC driving-vehicles have zero tailpipe emissions inside cities, which is of utmost importance for human-health protection.

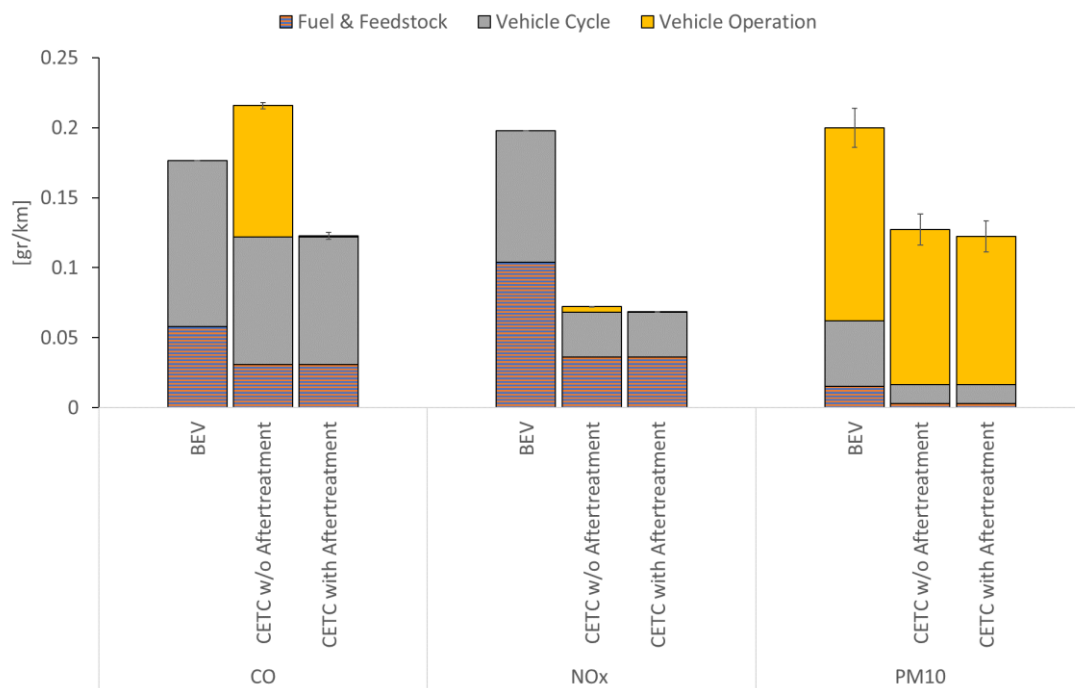


Figure 6 – Air quality impact comparison between BEV and CETC driven vehicles with and without exhaust aftertreatment

Air-quality impact comparison clearly demonstrates substantially lower air pollution levels of the CETC driven-vehicle with exhaust gas aftertreatment compared to BEV. Moreover, even without aftertreatment CETC outperforms BEV in terms of NO_x

and PM because of the ultra-low engine-out NO_x emissions when the ICE is fed with a hydrogen-rich reformat [18] and a low share (~10% [43]) of exhaust particles in the total PUT PM emission. CETC's NO_x emission is very low due to the presence of CO₂ in the ICE cylinder, reducing the combustion temperature and mitigating NO_x formation. The most harmful impact to air quality is PM formation due to two reasons. First, most of PM formation results from the vehicle's operation phase, including tire, road and brake wear, which take place inside cities as well [43, 44]. Second, PM emissions are considered as the most harmful air pollutant for human health and are classified as class 1 pollutant by the WHO [45]. As BEVs are heavier, their PM formation in the operation phase is higher compared to the CETC driven vehicle.

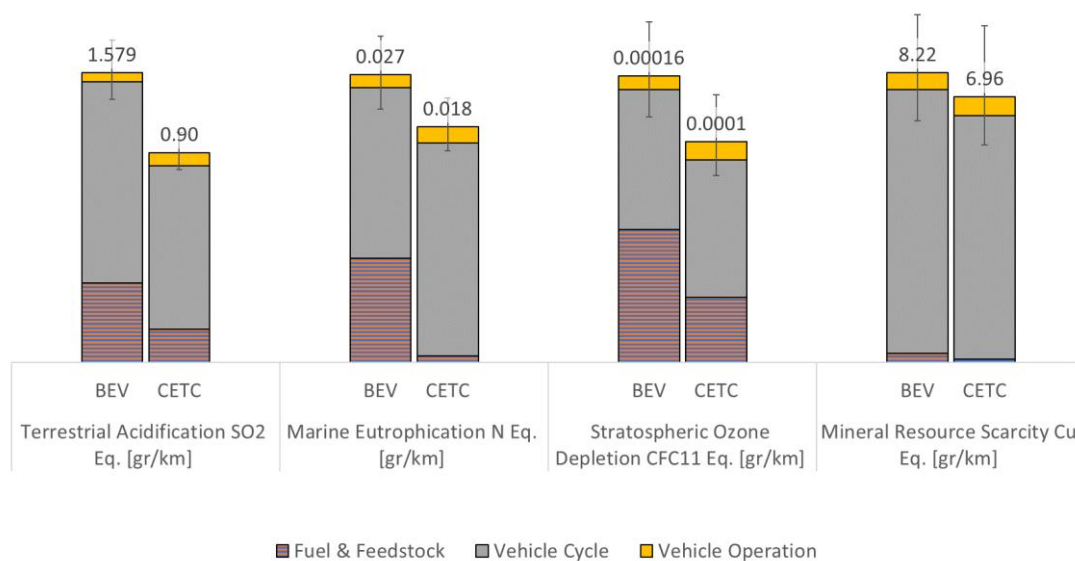


Figure 7 –Selected ecological impacts comparison between BEV and the CETC vehicle according ReCiPe 2016 Midpoint (H) [34].

Besides air-quality, other ecological impacts were analyzed using midpoint life-cycle impact-assessment metrics, following ReCiPe 2016 Midpoint (H) [34] (Fig. 7).

The results are unequivocally in favor of the CETC powertrain. Terrestrial acidification and mineral resource scarcity are higher for the BEV due to the greater use of copper and other materials that are required in the manufacturing process. Spoil from mining causing water eutrophication and coal mining for the electricity production of the BEV are responsible for the gap in the fuel & feedstock phase. Stratospheric ozone depletion is caused mainly by the release of refrigerants into the atmosphere and the emission of nitrous oxide (N₂O). The natural-gas transportation by pipelines to the electrical plants for BEV electricity production (~40%) and to the methanol production plants for the CETC methanol (100%) requires compressing and

cooling. Yet, around 20% of electricity in the US is produced by burning coal, which contributes approximately to two times more to the stratospheric ozone depletion than natural gas transport by nitrous-oxide emissions.

The main contributor for most of the ecological impacts analyzed in Fig. 7 is the vehicle cycle phase. Thus, a breakdown of this phase for the components manufacturing of the vehicles was conducted (Fig. 8), with a disaggregation of the production phase contributions for manufacturing of the vehicles.

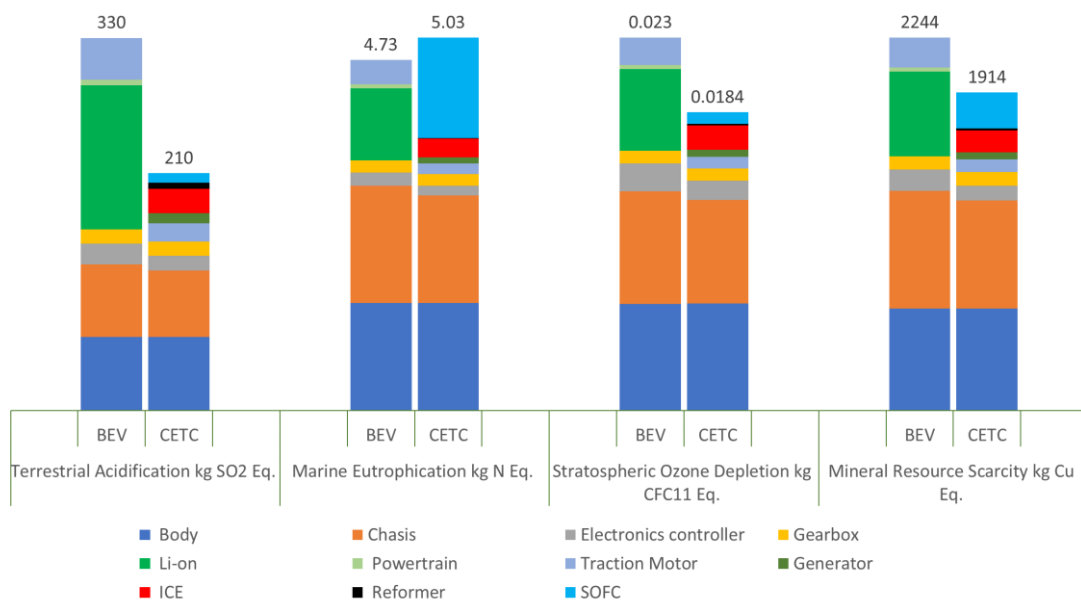


Figure 8 - Breakdown of the production phase to different components manufacturing for selected ecological impacts.

The production of the Li-on battery is the main cause for the disparity in favor of the CETC driven-vehicle (Fig. 8). This result is consistent with published LCA analyses of BEVs [1-7]. The only category in which the CETC powertrain is inferior in the production phase is the marine eutrophication category. The reason is the high amount of chromium steel used for the interconnect part of the SOFC [30].

In Fig. 9 a summary is presented for the various environmental impacts that were examined. The impacts are categorized by global-warming contribution (GHG emissions), ecological impacts, air quality and human toxicity, which is related to the use of carcinogenic and non-carcinogenic materials.

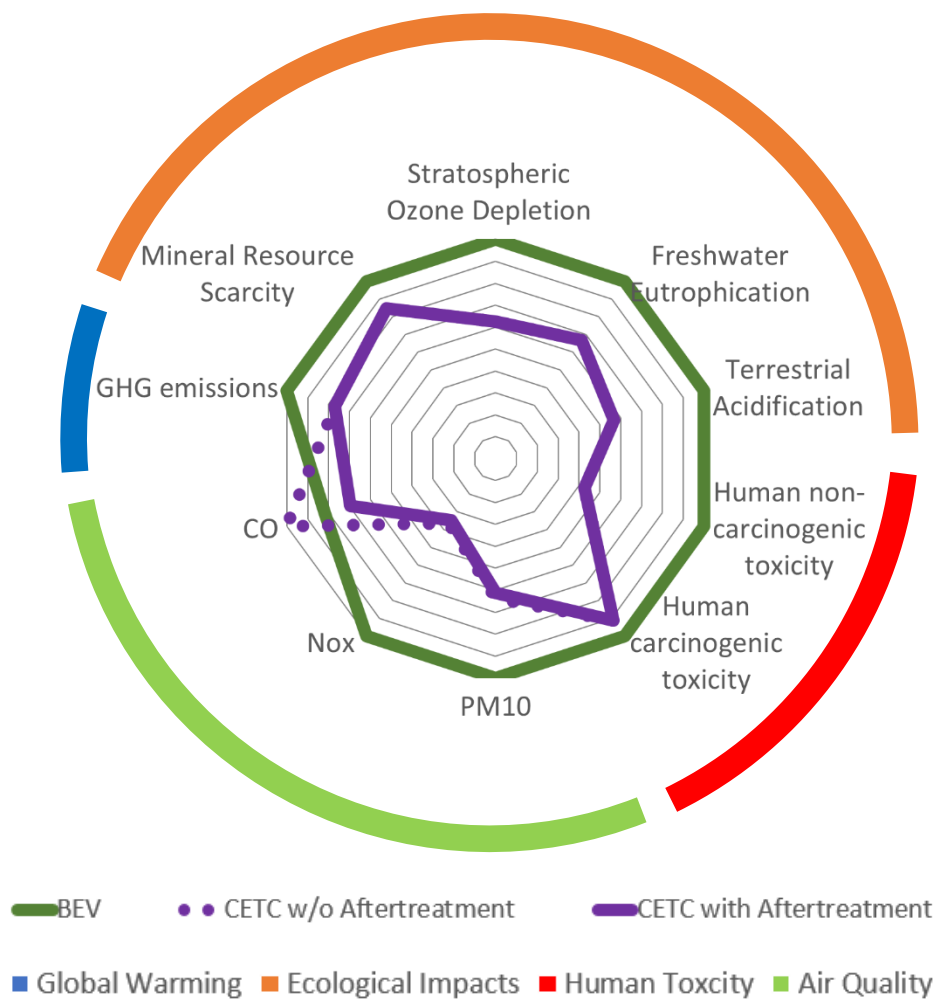


Figure 9 – Overall environmental impacts comparison between BEV and CETC vehicles, with and without aftertreatment.

Fig. 9 illustrates the advantageous environmental performance of the CETC vehicle compared to the BEV. This study avoids weighting each category to calculate the overall environmental impact by a single impact score, because all weighting methods involve human judgment and additional assumptions. Regardless, the CETC's environmental advantage over BEV is clear.

3.2 Commercialization challenges

Notably, BEVs have been successfully commercialized, and their price is reducing constantly. Here, we posit that the main challenge for the CETC powertrain commercialization is the adaption of the SOFC for transportation use. Modern commercial SOFCs withstand thousands of hours of use [38], which is sufficient for the

lifecycle of the selected case study or similar uses. However, these SOFCs can only withstand hundreds of thermal cycles due to thermal expansion at high working temperature [38], which is clearly not enough for ground transportation with its frequent startups and stops.

We believe that solutions to this main issue will be developed in the near future. For example, a relatively low-temperature SOFC is currently being developed (300-400°C) [46]. This temperature range still allows waste heat utilization for TCR, while making SOFC much less sensitive to thermal regime variations.

Apart from the SOFC thermal cycle durability, the other challenges are relatively easy to overcome. SOFC can safely operate with hydrogen-rich reformat [47] while the fuel reforming process is being commercialized and even optimized for transportation use [31, 32]. The standard ICE can be adopted easily to reformat fuel [39, 48] where the main necessary adaptations are the addition of a gaseous injector [48], and calibration of injection and ignition strategies. Warming up the reformer and the SOFC in cold-starts can be done by starting the ICE first either with the primary fuel - which would result in high emissions at the cold-start interval - or, by using a sufficient amount of on-board stored reformat for that interval.

4. Conclusions

Before concluding and elaborating on the feasibility of the proposed powertrain to compete with the electrical powertrain, it should be noted that most of the assumptions employed in the calculations are favorable towards the BEV. These include, among other, ignoring the impacts of infrastructure building for the technologies, as discussed earlier.

The results of the LCA show clearly that the CETC powertrain outperforms the battery-electric one. The CETC emits less GHG, is responsible for less air pollution and has lower ecological impacts. The overall energy demand from well-to-wheel is lower for the CETC-driven vehicle. Notably, electricity may be produced with reduced GHG emissions using renewable energy sources. However, methanol can also be produced using renewable technologies with CO₂ capturing, which would result again in an advantage for the CETC powertrain over BEV. In the production phase, the main source of disparity is due to battery production in the BEV, necessitating substantial technological development to bridge this gap.

Regarding air pollution and ecological impacts, the advantage of the CETC powertrain is even clearer. The main reasons for this are the weight difference that is

in favor of the CETC powertrain (higher consumption of materials and energy use in BEV production), and the complexity of battery production, which is highly intensive in resources such as lithium, copper, cobalt and more [42].

The hybrid configuration of the CETC powertrain enables the utilization of the relative advantages of the FC and ICE technologies involved. The FC operates solely inside the city, allowing for zero tailpipe emissions and high efficiency. The ICE operates only in the following cases: (i) cold-starts thus enabling SOFC and reformer warm-up, and (ii) high power demanding driving segments, mainly outside cities. Notably, ICE vehicles suffer from a significant efficiency drop in the low-power demanding segments, whereas FC vehicles suffer from a heavy powertrain that is necessary to meet the vehicle maximal power requirement. The CETC powertrain overcomes these challenges and maximizes the benefits of each subsystem.

CETC powertrain have some commercialization challenges, whereas the main challenge is the SOFC low thermal-cycles durability. However, we believe that this technological challenge, as the other commercial challenges will be resolved in the near future.

References

- [1] Xia, Xiaoning, and Pengwei Li. "A review of the life cycle assessment of electric vehicles: Considering the influence of batteries." *Science of The Total Environment* (2022): 152870.
- [2] Wu, Ziyang, Can Wang, Paul Wolfram, Yaxin Zhang, Xin Sun, and Edgar Hertwich. "Assessing electric vehicle policy with region-specific carbon footprints." *Applied Energy* 256 (2019): 113923.
- [3] Helmers, Eckard, Johannes Dietz, and Susanne Hartard. "Electric car life cycle assessment based on real-world mileage and the electric conversion scenario." *The International Journal of Life Cycle Assessment* 22, no. 1 (2017): 15-30.
- [4] Haugen, Molly J., Leonardo Paoli, Jonathan Cullen, David Cebon, and Adam M. Boies. "A fork in the road: Which energy pathway offers the greatest energy efficiency and CO2 reduction potential for low-carbon vehicles?" *Applied Energy* 283 (2021): 116295.
- [5] Bicer, Yusuf, and Ibrahim Dincer. "Comparative life cycle assessment of hydrogen, methanol and electric vehicles from well to wheel." *International Journal of Hydrogen Energy* 42, no. 6 (2017): 3767-3777.
- [6] Küfeoğlu, Sinan, and Dennis Khah Kok Hong. "Emissions performance of electric vehicles: A case study from the United Kingdom." *Applied Energy* 260 (2020): 114241.
- [7] Yang, Zijun, Bowen Wang, and Kui Jiao. "Life cycle assessment of fuel cell, electric and internal combustion engine vehicles under different fuel scenarios and driving mileages in China." *Energy* 198 (2020): 117365.
- [8] Helmers, Eckard, Johannes Dietz, and Martin Weiss. "Sensitivity analysis in the life-cycle assessment of electric vs. combustion engine cars under approximate real-world conditions." *Sustainability* 12, no. 3 (2020): 1241.
- [9] Girardi, Pierpaolo, Alessia Gargiulo, and Paola Cristina Brambilla. "A comparative LCA of an electric vehicle and an internal combustion engine vehicle using the appropriate power mix: the Italian case study." *The International Journal of Life Cycle Assessment* 20, no. 8 (2015): 1127-1142.
- [10] Lewis, Anne Marie, Jarod C. Kelly, and Gregory A. Keoleian. "Vehicle lightweighting vs. electrification: life cycle energy and GHG emissions results for diverse powertrain vehicles." *Applied Energy* 126 (2014): 13-20.

- [11] Bartolozzi, I., F. Rizzi, and Marco Frey. "Comparison between hydrogen and electric vehicles by life cycle assessment: A case study in Tuscany, Italy." *Applied Energy* 101 (2013): 103-111.
- [12] Pipitone, Emiliano, Salvatore Caltabellotta, and Leonardo Occhipinti. "A Life Cycle Environmental Impact Comparison between Traditional, Hybrid, and Electric Vehicles in the European Context." *Sustainability* 13, no. 19 (2021): 10992.
- [13] Marmiroli, Benedetta, Mattia Venditti, Giovanni Dotelli, and Ezio Spessa. "The transport of goods in the urban environment: A comparative life cycle assessment of electric, compressed natural gas and diesel light-duty vehicles." *Applied Energy* 260 (2020): 114236.
- [14] Choi, Wonjae, Eunji Yoo, Eunsu Seol, Myoungsoo Kim, and Han Ho Song. "Greenhouse gas emissions of conventional and alternative vehicles: Predictions based on energy policy analysis in South Korea." *Applied Energy* 265 (2020): 114754.
- [15] Naeini, Mina, James S. Cotton, and Thomas A. Adams II. "Dynamic life cycle assessment of solid oxide fuel cell system considering long-term degradation effects." *Energy Conversion and Management* 255 (2022): 115336.
- [16] Strazza, Carlo, Adriana Del Borghi, Paola Costamagna, Michela Gallo, Emma Brignole, and Paola Girdinio. "Life Cycle Assessment and Life Cycle Costing of a SOFC system for distributed power generation." *Energy Conversion and Management* 100 (2015): 64-77.
- [17] Boretti, Alberto. "Renewable hydrogen to recycle CO₂ to methanol." *International Journal of Hydrogen Energy* 38.4 (2013): 1806-1812.
- [18] Tartakovsky L., Sheintuch M. Fuel reforming in internal combustion engines. *Prog. Energy Combust Sci* 2018;67:88–114. <https://doi.org/10.1016/j.pecs.2018.02.003>.
- [19] Zabihian, F. and A. Fung. A Review on Modeling of Hybrid Solid Oxide Fuel Cell Systems. *International Journal of Engineering* 2009, 3.2, 85-119.
- [20] Winkler, W.; Nehter P.; Williams, M. C.; Tucker, D., and Gemmen, R. General fuel cell hybrid synergies and hybrid system testing status. *Journal of Power Sources* 2006, 159(1), 656-666.
- [21] Diskin, David, and Leonid Tartakovsky. "Finite-time energy conversion in a hybrid cycle combining electrochemical, combustion and thermochemical recuperation processes." *Energy Conversion and Management* 262 (2022): 115673.
- [22] Diskin, David, and Leonid Tartakovsky. "Efficiency at maximum power of the low-dissipation hybrid electrochemical–Otto cycle." *Energies* 13, no. 15 (2020): 3961.
- [23] Diskin D., and Tartakovsky L., Power and Efficiency Characteristics of a Hybrid Electrochemical-ICE Cycle. *SAE Int. J. Adv. & Curr. Prac. in Mobility* 2021, 3(4): 1487-1494. doi: 10.4271/2021-01-0230.
- [24] ISO 14040, Environmental Management - Life Cycle Assessment – Principles and Framework. International Organization for Standardization; 2006.
- [25] ISO 14044, Environmental Management - Life Cycle Assessment – Principles and Framework. International Organization for Standardization; 2006.
- [26] Argonne National Laboratory 2022 GREET 1 Model. <https://greet.es.anl.gov/>
- [27] Argonne National Laboratory 2022 GREET 2 Model. <https://greet.es.anl.gov/>
- [28] Wernet, G., Bauer, C., Steubing, B., Reinhard, J., Moreno-Ruiz, E., & Weidema, B. (2016). The ecoinvent database version 3 (part I): overview and methodology. *The International Journal of Life Cycle Assessment*, 21, 1218-1230.
- [29] Hula, A., Maguire, A., Bunker, A., Rojeck, T., & Harrison, S. (2021). *The 2021 EPA Automotive Trends Report: Greenhouse Gas Emissions, Fuel Economy, and Technology since 1975* (No. EPA-420-R-21-023)..
- [30] Teixeira Taboada, S. Life Cycle Assessment of solid oxide fuel cell systems for data centers A comparative study between three fuel alternatives: natural gas, biogas, and hydrogen. 2022. Master's thesis in Industrial Ecology, Chalmers University of Technology.
- [31] Sall, Erik D., David A. Morgenstern, James P. Fornango, James W. Taylor, Nichilos Chomic, and Jennifer Wheeler. "Reforming of ethanol with exhaust heat at automotive scale." *Energy & Fuels* 27, no. 9 (2013): 5579-5588.
- [32] Fowler, J., Morgenstern, D., Sall, E., & Veinbergs, M. E. (2014). Integration of an E85 reforming system into a vehicle-ready package and project results. *SAE Technical Paper* 2014-01-1191.
- [33] Belcastro, Elizabeth Lynn. Life cycle analysis of a ceramic three-way catalytic converter. 2012. PhD Thesis. Virginia Tech.
- [34] Huijbregts, M. A., Steinmann, Z. J., Elshout, P. M., Stam, G., Verones, F., Vieira, M., & Van Zelm, R. (2017). ReCiPe2016: a harmonised life cycle impact assessment method at midpoint and endpoint level. *The International Journal of Life Cycle Assessment*, 22, 138-147.

- [35] Khalifa, Sherif A., Sabrina Spatari, Aaron T. Fafarman, and Jason B. Baxter. "Environmental sustainability of mixed cation perovskite materials in photovoltaics manufacturing." *ACS Sustainable Chemistry & Engineering* 8, no. 44 (2020): 16537-16548.
- [36] Kar, Saurajyoti, Rajveer Singh, Patrick L. Gurian, Adam Hendricks, Paul Kohl, Sean McKelvey, and Sabrina Spatari. "Life cycle assessment and techno-economic analysis of nitrogen recovery by ammonia air-stripping from wastewater treatment." *Science of The Total Environment* 857 (2023): 159499.
- [37] Bilich, Andrew, Kevin Langham, Roland Geyer, Love Goyal, James Hansen, Anjana Krishnan, Joseph Bergesen, and Parikhit Sinha. "Life cycle assessment of solar photovoltaic microgrid systems in off-grid communities." *Environmental Science & Technology* 51, no. 2 (2017): 1043-1052.
- [38] O'hayre, R., Cha, S. W., Colella, W., and Prinz, F. B., Fuel cell fundamentals; John Wiley & Sons, 2016.
- [39] Thawko, Andy, Amnon Eyal, and Leonid Tartakovsky. "Experimental comparison of performance and emissions of a direct-injection engine fed with alternative gaseous fuels." *Energy Conversion and Management* 251 (2022): 114988.
- [40] Sculley, Robert D. "Vehicle emission rate analysis for carbon monoxide hot spot modeling." *JAPCA* 39, no. 10 (1989): 1334-1343.
- [41] Chaim, Michael Ben, and Efraim Shmerling. "A Model for Vehicle Fuel Consumption Estimation at Urban Operating Conditions." *International Journal of Mechanics* 7 (2013): 18-23.
- [42] J.B. Dunn, L. Gaines, M. Barnes, J. Sullivan and M. Wang, 2012. "Material and Energy Flows in the Materials Production, Assembly, and End of Life Stages of the Automotive Lithium Ion Battery Life Cycle," ANL/ESD/12-3.
- [43] Liu, Ye, Haibo Chen, Ying Li, Jianbing Gao, Kaushali Dave, Junyan Chen, Tiezhu Li, and Ran Tu. "Exhaust and non-exhaust emissions from conventional and electric vehicles: A comparison of monetary impact values." *Journal of Cleaner Production* 331 (2022): 129965.
- [44] Timmers, Victor RJH, and Peter AJ Achten. "Non-exhaust PM emissions from electric vehicles." *Atmospheric Environment* 134 (2016): 10-17.
- [45] Hamra, Ghassan B., Neela Guha, Aaron Cohen, Francine Laden, Ole Raaschou-Nielsen, Jonathan M. Samet, Paolo Vineis et al. "Outdoor particulate matter exposure and lung cancer: a systematic review and meta-analysis." *Environmental Health Perspectives* (2014).
- [46] Lee, Yoon Ho, Ikwhang Chang, Gu Young Cho, Joonho Park, Wonjong Yu, Waqas Hassan Tanveer, and Suk Won Cha. "Thin film solid oxide fuel cells operating below 600 C: a review." *International Journal of Precision Engineering and Manufacturing-Green Technology* 5, no. 3 (2018): 441-453.
- [47] Aguiar, P. Adjiman C. S., and Brandon N. P., Anode-supported intermediate temperature direct internal reforming solid oxide fuel cell. I: model-based steady-state performance. *Journal of Power Sources* 2004, 138.1-2: 120-136
- [48] Poran, A., A. Thawko, A. Eyal, and L. Tartakovsky. "Direct injection internal combustion engine with high-pressure thermochemical recuperation—Experimental study of the first prototype." *International Journal of Hydrogen Energy* 43, no. 27 (2018): 11969-11980.