carculator: an open-source tool for prospective environmental and economic life cycle assessment of vehicles. When, Where and How can battery-electric vehicles help reduce greenhouse gas emissions?

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Abstract

This paper introduces *carculator*, a Python library to conduct environmental life cycle assessments and quantify total costs of ownership of current and future passenger vehicles. Because *carculator* is open-source and equipped with an easy-to-use online graphical user interface, it allows to produce context-specific results, deemed more relevant than results otherwise published in more static formats, such as reports. Besides conventional "static" analyses, *carculator* also allows for error propagation from input parameters, for several powertrains, vehicle size categories and fuel types, for any year between 2020 and 2050. Its applicability is exemplified with the analysis of the expected evolution of life-cycle greenhouse gas emissions per kilometer driven for gasoline-powered and battery electric vehicles between 2020 and 2050, for each member state of the European Union, plus the United Kingdom, Switzerland and Norway. Results show that, as soon as 2020, battery electric vehicles perform better than gasoline-powered vehicles in 28 out of the 30 countries considered.

Highlights

- Transparent life cycle assessment for current and future passenger vehicles
- Time-adjusted foreground and background inventories, from 2000 to 2050
- Driving cycle-based estimate for noise and hot pollutant emissions
- Error propagation analysis for current and future vehicles
- BEV already perform better than ICEV in 28 out of 30 countries in Europe

Keywords: Life Cycle Assessment (LCA), passenger vehicles, battery electric, mobility, projection, error propagation.

Abbreviations

Acronym	**Description**
BEV	Battery electric vehicle
CADC	Common Artemis driving cycles
FCEV	Fuel cell electric vehicle
GHG	Greenhouse gases
GWP	Global warming potential
HBEFA	Handbook emission factors for road transport
HEV	Hybrid electric vehicles
IAM	Integrated assessment model
ICEV	Internal combustion engine vehicle
LCA	Life cycle assessment
LFP	Lithium ferrophosphate battery
NCA	Lithium nickel cobalt aluminum oxide battery
NEDC	New European driving cycle
NMC	Lithium nickel manganese cobalt oxide battery
PHEV	Plug-in hybrid engine vehicle
WLTC	Worldwide harmonized light vehicles test cycles
WLTP	Worldwide harmonized light vehicles test procedure

1 Introduction

The European Commission recently announced the goal to achieve a “net-zero” Greenhouse Gas (GHG) emissions level by 2050 [1]. Currently, more than 20% of the EU’s GHG emissions are due to transport activities [2] and almost 50% of those are caused by passenger vehicles [3]. As opposed to other energy-intensive sectors, such as power generation and industry, emissions from transportation activities have been growing in the past years [2]. Therefore, effective measures to reduce these emissions are urgently needed.

The electrification of powertrains using battery electric vehicles (BEV) is seen as a promising option. However, BEV are not free of environmental burdens: while they offer the advantage of removing exhaust emissions, other aspects of their life cycle, such as the supply of electricity or the production of the vehicle frame and components, may still lead to substantial GHG emissions and other environmental impacts. Life Cycle Assessment (LCA) is a tool fit for characterizing such impacts along the life cycle of vehicles. Several recent LCA studies have shown that BEV substantially reduce life cycle GHG emissions compared to conventional internal combustion engine vehicles (ICEV) fueled with gasoline or diesel. This conclusion seems to hold true provided that the electricity supply is associated with low GHG emissions [4–26]. In contrast to such development, a few studies claimed that current BEV lead to higher GHG emissions than ICEV [27–29] in countries where most anlayses show the opposite. In addition, popular news articless raised doubts on the environmental performance of BEV [30–37]. These studies and news articles cause confusion among the general audience and decision-makers. The assumptions made in such studies are often ill-rooted, and rapidly exposed by the scientific community, as a press article demonstrates [38] in the case of the work byBuchal et al. [39]. Such phenomenon reveals an important aspect of LCA of BEV: in contrast to ICEV, much of the environmental performance of BEV depends on the complex modeling of upstream services in time and space, distant from the use phase of the vehicle, as well as some other parameters specific to the conditions of use of the vehicle. As such, LCA studies on passenger vehicles never fully fit a precise context as several sensitive parameters depend on the geography (e.g., the electricity mix used for charging the battery), on the temporal scope (e.g., weight reduction of the vehicle glider over time), while others can be depending on the behavior of the user (e.g., number of kilometers driven per year). This stresses the need for transparent and comprehensive LCA models able to adjust foreground and background inventories to deliver relevant results that fit a specific context. This largely fails to be commonplace nowadays among available LCA models of passenger vehicles.

Indeed, only a few prospective analyses with a parameterized temporal and geographical dimension exist. The few future-oriented studies available conclude that a reduction of the environmental burden of both BEV and ICEV should be expected due to improved technology performance, engine hybridization, and progressive integration of renewable sources of energy in the electricity supply for battery charging [5,8,22,24,40–43]. Three LCA studies of passenger vehicles have considered the effects of potential changes in the global economy, but all limited to the expected changes in the global power supply [21,22,44]. A fourth and more recent publication by Knobloch et al. [18] also attempts to include the effects of economy-wide changes in the power supply on the life cycle GHG emissions of BEV. It however leaves out the life cycle emissions of the power-producing technologies, using instead a regional average GHG emission factor based on direct emissions only. Yet, these studies concur on the importance of a shift from fossil fuel-based power plants to renewable energy technologies and its substantial effects on the burdens associated with material and energy supply chains and hence, overall LCA results. While this shows efforts to give a temporal and geographical dimension to the analysis, these studies result in a single context of use, making it difficult to use the results in other contexts (e.g., in another country, or with another driving cycle).

Therefore, this paper introduces *carculator*. It is an LCA library written with the programming language Python. It assesses the environmental and economic life cycle footprint of passenger vehicles by adjusting the inventories along time, geography and user-defined preferences, to provide a tailored basis for decision-making. Based on an open and well-documented source code, the tool offers transparency as to which input parameters are used and how results are calculated. *carculator* is designed to perform fast calculations while allowing the user to adjust the model to his or her own context of vehicle production, use and disposal. During the development of this tool, the following shortcomings identified in the body of literature were in focus:

- Key parameters of passenger vehicle models are not always easy to identify, nor are they always reported. Also, a sensitivity analysis on these key parameters is often lacking. In contrast to this, *carculator* offers a convenient function to perform one-at-a-time sensitivity analysis to identify the most influential parameters.
- Epistemic uncertainty in the input parameters and the model are often not addressed. *carculator* allows to quantify stochastic uncertainty in input parameters and characterize its propagation on end-results.
- Several studies are based on outdated information, but *carculator* relies on updated inventories for battery electric and fuel cell-based vehicles, as well as for a number of fuel pathways, for which the publication source and date are listed in the Electronic Supplementary Information document. Additionally, the source of each inventory, including their year of publication, is listed in the software documentation.

- In most studies, the electricity mix used to charge batteries or produce hydrogen is not time-distributed but instead corresponds to the year of the vehicle production. Given the number of years of use defined by the user, *carculator* produces instead a time-distributed electricity mix for battery charging and electrolysis-based hydrogen production.
- Comparisons of different drivetrains are often based on biased assumptions and input parameters. *carculator* does not prevent biases as such, but discloses them.
- Results from studies in the literature are hard to reuse as the inventories are not available or clearly described. *carculator* has several export functions, which allow to reuse the inventories in common LCA software, such as Brightway2 [45].
- Finally, few to no prospective studies adjust both the vehicle inventory and the background inventory over time to reflect progress in terms of material and energy use efficiency: *carculator* considers the expected progress in the automotive industry as well the penetration rate of renewable sources of energy in the electricity network of different regions of the world by coupling the life cycle inventory database ecoinvent [46] and the Integrated Assessment Model (IAM) REMIND [47,48] – although other IAMs could be used.

As a case study to demonstrate the capabilities of the calculation framework, this study quantifies country-specific climate change impacts, expressed in terms of GHG emissions per km, of BEV between 2020 and 2050, over those of its gasoline-powered counterpart. This analysis is based on several electricity supply scenarios (details provided in section 2.2.3), with varying degrees of climate policy ambition, both at the country level and globally. Hence, this case study aims to answer whether, when and under which conditions BEV provide benefits regarding potential climate change impacts in each Member State of the European Union, in addition to Switzerland, Norway and the United Kingdom.

2 Method

The structure of the tool can be described in terms of *foreground* and *background* models. The foreground model is concerned with calculating the physical attributes of the vehicles, such as the sizing of the vehicle components, the requirements in terms of motive energy as well as quantifying direct exhaust and non-exhaust emissions. The background modeling deals with the provision of upstream services necessary to support the life cycle of the vehicle. It generally includes the supply of fuel or electricity, the infrastructures, but also the provision of the different material fractions necessary to the manufacture and assembly of the vehicle components.

The next subsections describe in detail the method followed in the foreground and background models of *carculator.*

2.1 Vehicles foreground model

carculator is based on the source code initially used in the work of Cox et al. [21], which has been refactored into a Python library. It has been extended with the addition of several calculation modules (e.g., noise and exhaust emissions modelling), an improved handling of projected electricity mixes for battery charging, an increased range of vehicle production years to choose from, as well as a wider catalogue of powertrain and fuel types and pathways. These additional features are presented in the following sections. The calculation framework of *carculator* includes a large portfolio of powertrains, size categories, and years – see Table 1. They represent up to 3,150 unique vehicle configurations (9 powertrains x 7 size categories x 50 production years), in addition to numerous fuel pathways, stored in a four-dimensional numerical array: *powertrain*, *size*, *year* and *parameter*, where the dimension *parameter* stores *input* and *calculated* parameters.

Table 1 Powertrain and size categories, and year of production offered by *carculator*

Powertrain	**Fuel pathways**	**Size**	**Year**
Internal combustion engine vehicle, diesel-powered (ICEV-d), including a mild engine hybridization in the future	Conventional diesel, bio-diesel (from micro-algae as well as used cooking oil) and synthetic diesel (from hydrogen).	Mini,Small, Lower, medium Medium, Large, SUV, Van	2000 to 2050
Internal combustion engine vehicle, gasoline-powered (ICEV-p), including a mild engine hybridization in the future	Conventional gasoline, bio-ethanol (from maize starch, sugar beet, forest residues and wheat straw) and synthetic gasoline (from methanol).		
Internal combustion engine vehicle, compressed natural gas-powered (ICEV-g), including a mild engine hybridization in the future	Compressed natural gas, bio-methane (from livestock manure), synthetic methane.		
Battery electric vehicle (BEV)	Over 80 country-specific electricity mixes.		
Hybrid electric gasoline-powered vehicle (HEV-p)	Hydrogen from electrolysis, from steam methane reforming of natural gas, biogas, as well as from coal gasification.		
Hybrid electric diesel-powered vehicle (HEV-d)			
Plug-in hybrid electric gasoline-powered vehicle (PHEV-p)			
Plug-in hybrid electric diesel-powered vehicle (PHEV-d)			

FCEV (hydrogen fuel cell)

Operations are performed based on *input* parameter values to obtain *calculated* parameter values. For example, the calculated parameter *power* (i.e., the required power output of an engine) is defined by the following relation:

$$power\ [kW] = \frac{\left(power - to - mass\ ratio\ \left[\frac{W}{kg}\right] * curb\ mass[kg]\right)}{1000\ [W/kW]}$$

Here, *power-to-mass ratio* is an *input* parameter, while *curb mass* is another *calculated* parameter. Input parameter values are initially given for current and future vehicles, along with uncertainty information (i.e. uncertainty information is represented by a distribution type and parameters). To continue this example, the input parameter *power-to-mass* ratio is defined as:

```
"22-2017-power to mass ratio": {
  "amount": 60.0,
  "category": "Glider",
  "kind": "distribution",
  "loc": 60.0,
  "maximum": 90.0,
  "minimum": 40.0,
  "name": "power to mass ratio",
  "powertrain": [
    "BEV",
    "FCEV",
    "HEV-p",
    "ICEV-d",
    "ICEV-g",
    "ICEV-p",
    "PHEV-c",
    "PHEV-e"
  ],
  "sizes": [
    "Mini"
  ],
  "source": "Hirschberg et al. (2016), Grunditz, Thiringer (2016), VCS (2018)",
  "uncertainty_type": 5,
  "unit": "W/kg",
  "year": 2017
}
```

This input parameter applies to all powertrains of the size class “Mini” for the current period. Its value is defined by a triangular distribution with a minimum-maximum of 40-90 W/kg and centered around 60 W/kg. Values for input parameters are originally defined for the current period as well some period in the future, corresponding approximately to 2040. By means of linear interpolation between the current and future input parameters based on a first degree polynomial function, vehicles can be reasonably modeled for any production year between 2000 and 2050. While it is possible to extrapolate vehicle models beyond 2050, the results would be highly uncertain as data with such a temporal scope is lacking.

Seven modules are used to obtain all the different calculated parameter values:

- the driving cycle module,
- the mass module,
- the auxiliary energy module,
- the motive energy module,
- the noise emissions module,
- and the exhaust emissions module.

An overview of the modules and how they relate to one another is given in the Electronic Supplementary Information document.

All the input and calculated parameters can be accessed and modified, should the default values provided seem inappropriate for the scope of analysis, or simply for the purpose of sensitivity analysis. This can range from modifying the number of passengers in the vehicle down, to adjusting the charge and discharge efficiency rate of the battery of a BEV or the engine hybridization level of future ICE vehicles (i.e., the share of the overall power output of a powertrain provided by an electric engine).

2.1.1 A functional unit based on the driving cycle

The functional unit of the model is the driving distance of 1 kilometer, given a user-specified driving cycle. The concept of driving cycle, which defines the speed level of the vehicle for every second of driving, is central to the foreground model. The driving cycle characterizes the conditions of driving, sets the requirements in terms of acceleration and is the basis for calculating noise and exhaust emissions. Calculated parameters obtained from the driving cycle are defined in Figure 1.

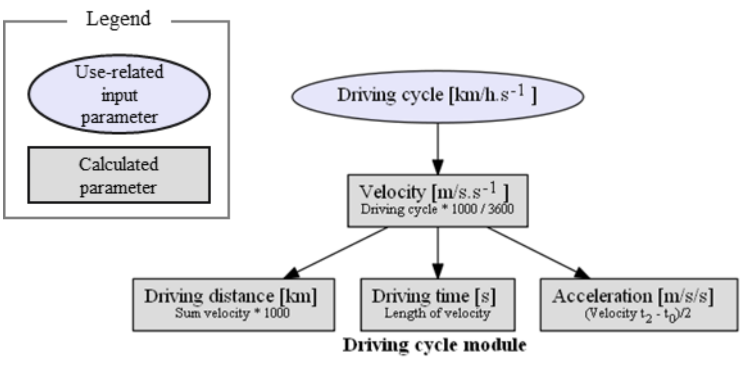


Figure 1 Parameters calculated from the driving cycle

The relation between the driving cycle and the required motive energy is illustrated in Figure 2, where the driving distance, velocity and acceleration are used to calculate the kinetic and aerodynamic energy requirements.

The tool offers the choice between the driving cycles described in Table 2.

Table 2 Characteristics of driving cycles available in *carculator*

	WLTC	**WLTC 3.1**	**WLTC 3.2**	**WLTC 3.3**	**WLTC 3.4**	**CADC Urban**	**CADC Road**	**CADC Motorway**	**CADC Motorway 130**	**CADC**	**NEDC**
Environment type	Urban, suburban and motorway	Urban	Suburban	Motorway	Motorway	Urban	Suburban	Motorway	Motorway	Urban, suburban and motorway	Urban, suburban and motorway
Driving time [s]	1,801	590	433	455	323	994	1,082	1,068	1,068	3,144	1,201
Driving distance [km]	23	3	5	7	8	5	17	30	29	52	11
Average speed [km.h^{-1}]	46	19	40	57	92	18	57	100	97	59	33
Average positive acceleration [m.s^{-2}]	0.51	0.55	0.53	0.58	0.37	0.7	0.53	0.43	0.42	0.55	0.51
Idling time [s]	235	150	48	30	4	283	33	16	16	332	314

Additionally, the tool also accepts user-defined driving cycles as well as road gradients.

The motive energy is summed together with the auxiliary energy, which is the energy required to operating the heating and cooling systems of the vehicles as well as the onboard electronics, to obtain the *tank-to-wheel* energy consumption of a vehicle given a specified driving cycle.

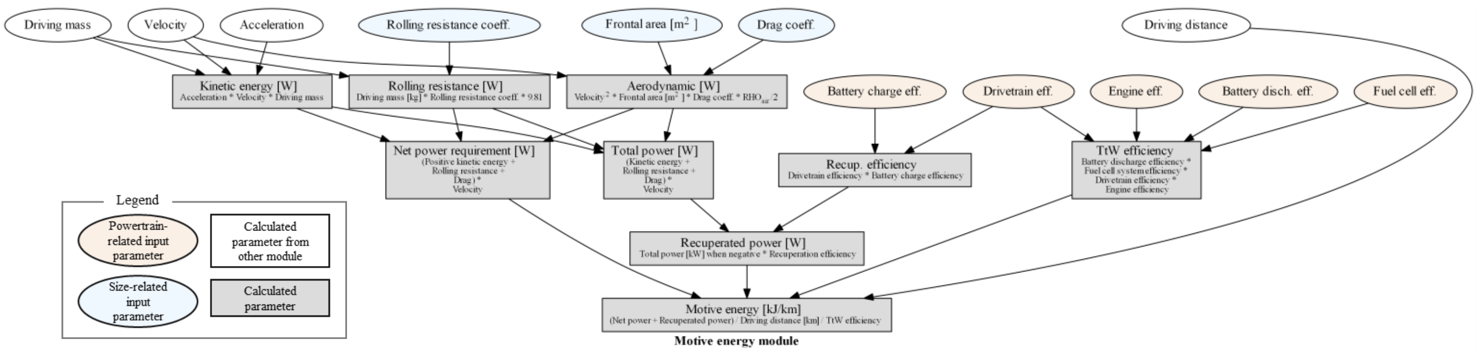


Figure 2 Motive energy calculation module

The driving cycle is also used to calculate exhaust emissions for current vehicles with internal combustion engines. The Handbook Emission Factors for Road Transport (HBEFA) database 4.1 [49], which provides emission factors based on engine maps created from emission measurements, shows the relation between speed level and emission of pollutants. *carculator* uses this relation to quantify the amount of pollutants emitted along the driving cycle for vehicles with the EURO 6-d pollution class – which is an updated implementation of the EURO 6 pollution class with emission measurements performed on more realistic driving conditions –, as illustrated in Figure 3 for a gasoline-fueled vehicle. Additionally, an uncertainty range (i.e., yellow-shaded area in Figure 3) representing a correction factor of 1.43 is considered, to include deviations observed between emissions under the WLTP test and real driving emissions [50]. Therefore, vehicles modelled in *carculator* comply with the EURO 6d emission limits, provided that the WLTC driving cycle is selected. Yet, this does not mean that the calculated emissions would remain below the limit set by the EURO 6d pollution class under different driving conditions (i.e., a different driving cycle, a higher cargo mass, etc.), nor does it not imply that emissions under real driving conditions are below that limit. Also, the relation between nitrous oxide (N_2O) and ammonia (NH_3) emissions and speed level is not convincing. In fact, these two components seem rather related to the temperature of the catalyst, which can be reflected by the traffic situation, as illustrated in Figure 4. Therefore, for these two pollutants, the average value observed across the different traffic situations is used, instead of their relation to the speed level.

If the user chooses one of the eleven driving cycles proposed by *carculator*, the environment types defined for that driving cycle (see Table 2) are used to further specify emissions for the urban, suburban and rual inventory compartments, respectively. Alternatively, if the user provides a custom driving cycle, speed level intervals are used to compartmentalize emissions:

- pollutants emitted at a speed level comprised between 0 and 50 km/h are assumed to be released in an urban inventory compartment,
- pollutants emitted at a speed level comprised between 51 and 80 km/h are assumed to be released in a suburban inventory compartment,
- and pollutants emitted at a speed level superior to 80 km/h are assumed to be released in a rural inventory compartment.

This allows to use compartment-specific characterization factors – mostly relevant for toxicitiy-related impact categories – at the impact assessment level.

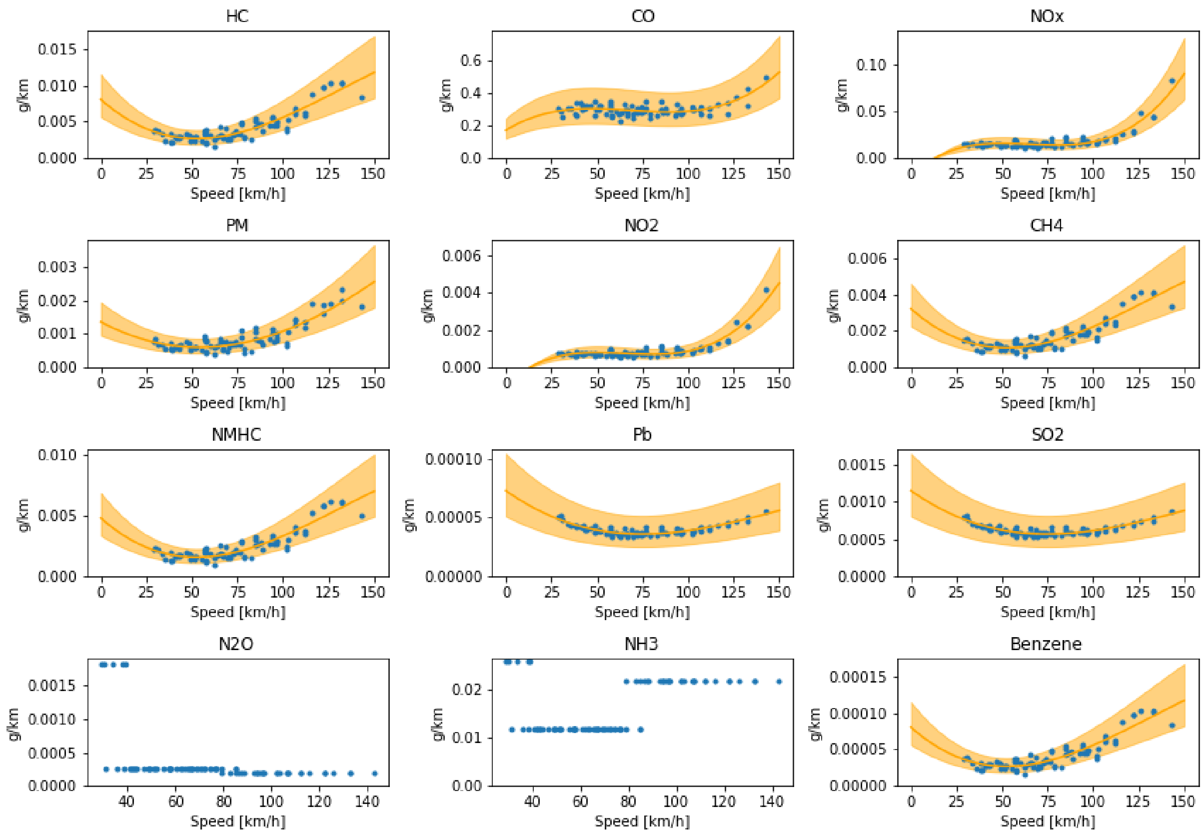


Figure 3 Relation between speed level and exhaust emissions for a gasoline-fueled vehicle. Blue dots: emission values modelled by HBEFA 4.1. Orange line: linear regression used by *carculator* as best-guess value. Yellow shaded area: minimum-maximum value range used for error propagation analyses. Data source: HBEFA 4.1 [49]

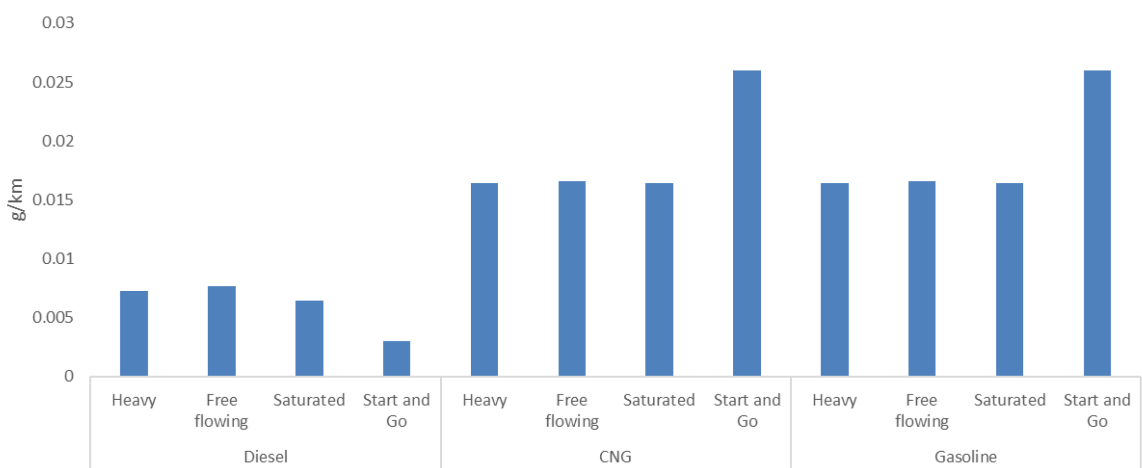


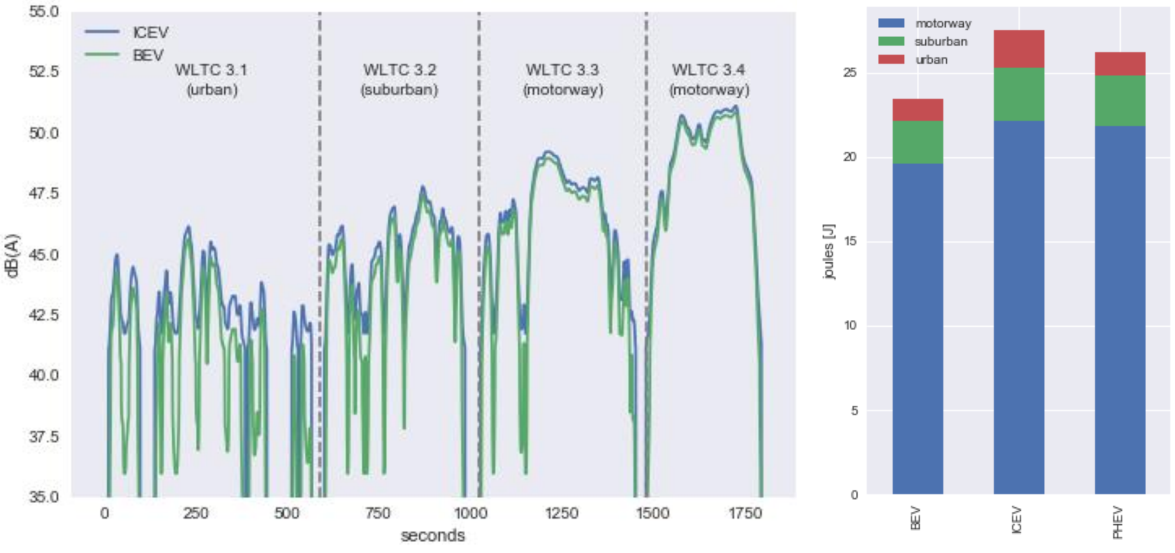
Figure 4 Relation between ammonia (NH_3) emissions and traffic situations for EURO 6d diesel, gas and gasoline-fueled vehicles. Data source: HBEFA 4.1 [49]

carculator does not assume a reduction of those emissions in the future, simply because no study or data seem to be supporting that claim. Rather, a hybridization of the powertrain of ICE vehicles is assumed, which allows to use a smaller engine that operates a greater percent of the time at full power, thereby increasing the efficiency of the powertrain.

Finally, the driving cycle is also an important input parameter to the noise emissions model used by *carculator*. Noise levels (in dB) are calculated for eight frequency ranges for each second of the driving cycle to obtain propulsion and rolling noise levels, based on coefficients developed from the CNOSSOS project [51]. However, this model has several limitations. One of them is that it does not differentiate noise emission levels within the different types of ICEV (i.e., diesel, gasoline, compressed natural gas) or size categories. For electric engines, special coefficients apply [52]. Also, electric vehicles are added a warning signal of 56 dB at speed levels below 20 km/h. Finally, hybrid vehicles are assumed to use an electric engine up to a speed level of 30 km/h, beyond which the combustion engine is used. The sum of the propulsion and rolling noise levels is converted to noise power (in joules) and divided by the distance driven to obtain the noise power per km driven (joules/km), for each frequency range.

Figure 5.a illustrates a comparison of noise levels between an ICEV and BEV as calculated by the tool, over the driving cycle WLTC. In this figure, the noise levels at different frequency ranges have been summed togeter to obtain a total noise level (in dB), and converted to dB(A) using using the A-weighting correction factor, to better represent the "loudness" or discomfort to the human ear. Typically, propulsion noise emissions dominate in urban environments (which corresponds to the section 3.1 of the driving cycle), thereby justifying the use of electric vehicles in that regard. This is represented by the difference between the ICEV and BEV lines in the section 3.1 of the driving cycle in Figure 5.a. The difference in noise level between the two powertrains diminishes at higher speed levels (see sections 3.2, 3.3 and 3.4) as rolling noise emissions dominate above a speed level of approximately 50 km/h. This can be seen in Figure 5.b, which sums up the sound energy produced, in joules, over the course of the driving cycle.

Noise emissions are further disaggregated into urban, sub-urban and rural inventory compartments, following the method used to compartmentalize exhaust emissions described earlier. The study from Cucurachi and Heijungs (2014) provides compartment-specific noise emission characterization factors against midpoint and endpoint indicators – expressed in Person-Pascal-second and Disability-Adjusted Life Year, respectively.



a) b)

Figure 5 a) Noise emission level comparison between ICEV and BEV, based on the driving cycle WLTC. b) – Summed sound energy comparison between ICEV, BEV and PHEV, over the duration of the WLTC driving cycle.

2.1.2 Sizing of vehicles

Another important calculated parameter to define the motive energy is the curb mass, which is the mass of the vehicle in driving order, but without passengers or cargo. The model sizes the different vehicle components. This includes the mass of the fuel tank, the glider, the engine, etc. The sum of the mass of these components, in addition to the mass of the passengers and cargo, amounts to the *driving mass*. The driving mass calculated, the model defines the requirements in terms of engine power and engine mass, themselves feeding back into the calculation of the driving mass. This iterative work is performed until the driving mass of the vehicle stabilizes. While the driving mass could instead be exogenously given, this bottom-to-top approach provides a granularity at the component level, which is then validated against external sources (i.e., passenger vehicles database).

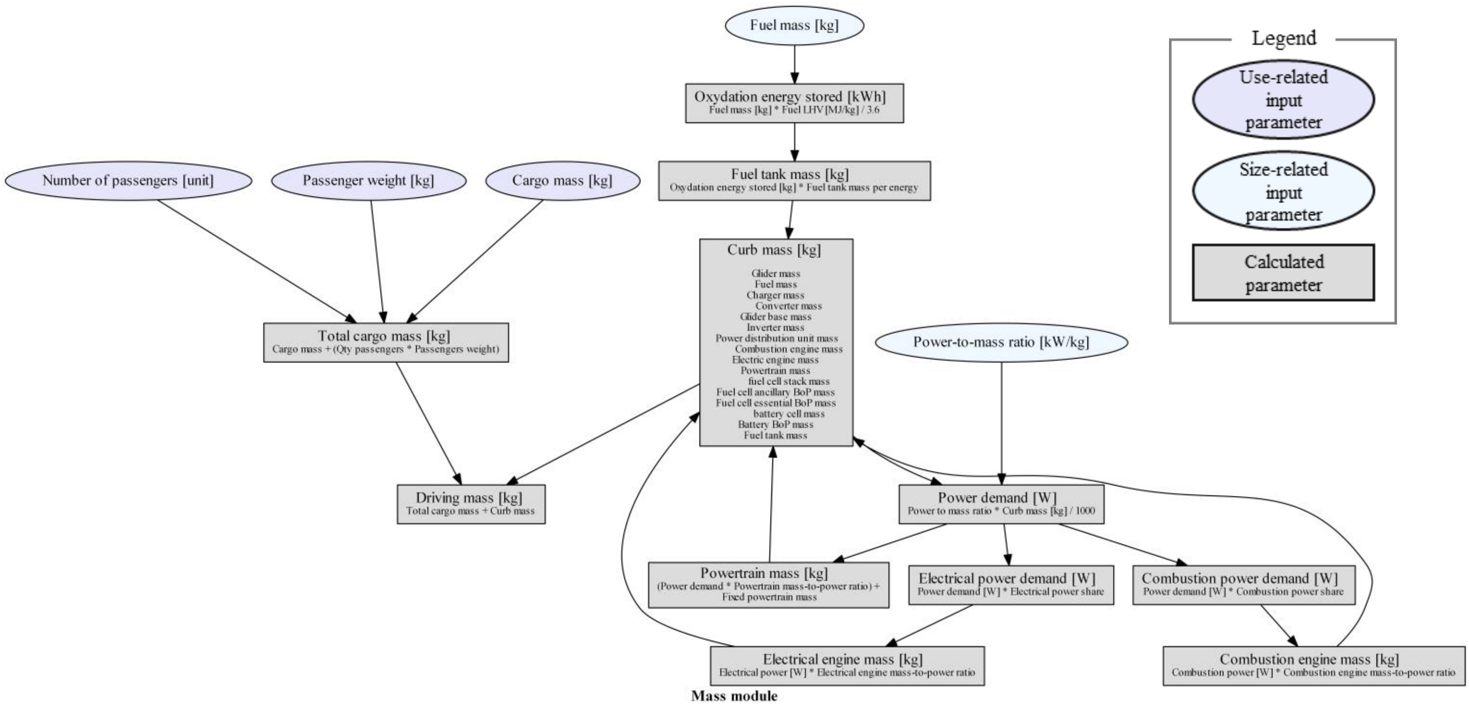


Figure 6 Vehicle mass module

2.1.3 Validation

The curb mass calculated by the model for current vehicles is validated against a database of passenger vehicles [54]. A selection of 11,585 passenger vehicles manufactured from 2015 until today are selected. The calibration of the curb mass is shown in Figure 7.

Also, the validity of the tank-to-wheel energy consumption for current vehicles is confirmed by comparing it against measurement data provided by the European monitoring program of CO_2 emissions for passenger vehicles [55]. The objective of this monitoring program is to record a number of data points, including tank-to-wheel energy consumption based on the WLTC driving cycle, for each vehicle newly registered in the European Union. The validation is performed against 15,272,915 measurement points for the tank-to-wheel energy consumption, grouped and averaged over 6,965 vehicle models. The result of this validation is shown in Figure 8. It seems that *carculator* overestimates the tank-to-wheel energy consumption for the lower size classes (i.e., Mini, Small and Lower medium) of plugin hybrid (PHEV) powertrains. This may be due to a higher percentage of the range being powered by the electric engine, as smaller vehicles tend be used for shorter trips and mostly in urban areas.

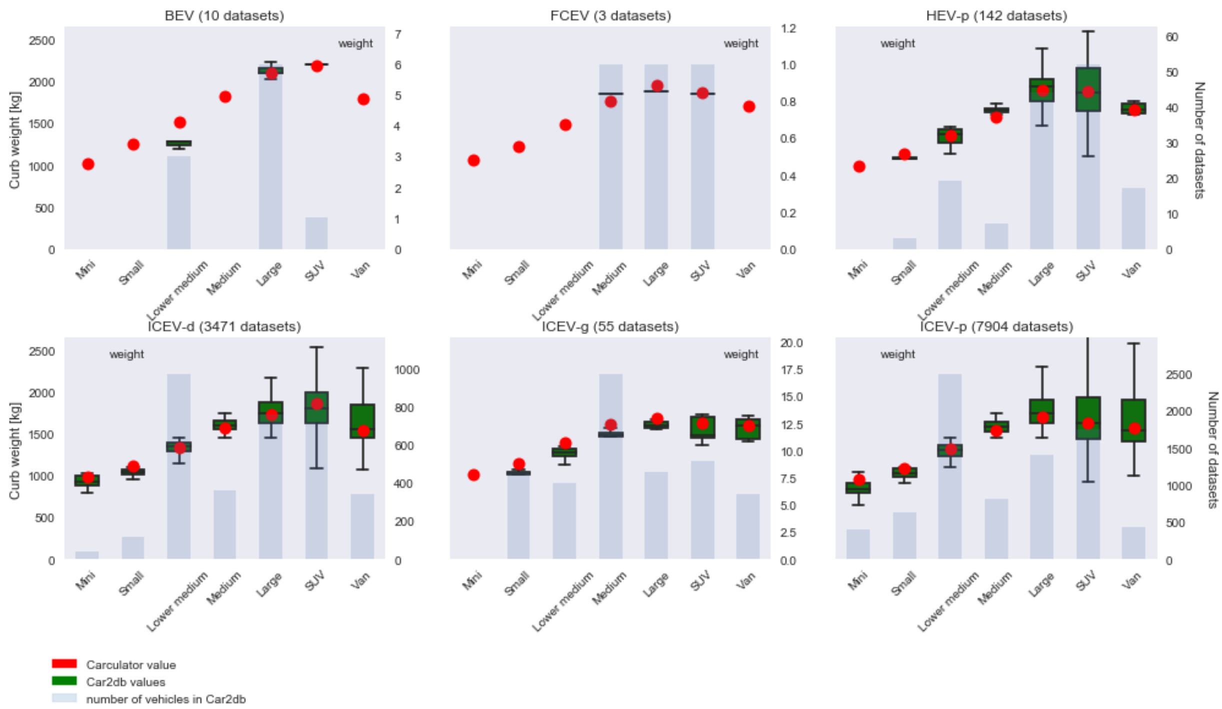


Figure 7 Validation of the curb mass against the datasets from the passenger vehicles database Car2db. Horizontal lines within the green boxes represent the median value. The green boxes represent 50% of the distribution (25th-75th percentiles). The whiskers represent 90% of the distribution (5th-95th percentiles). Outliers are not shown. Source for vehicle datasets: [56]

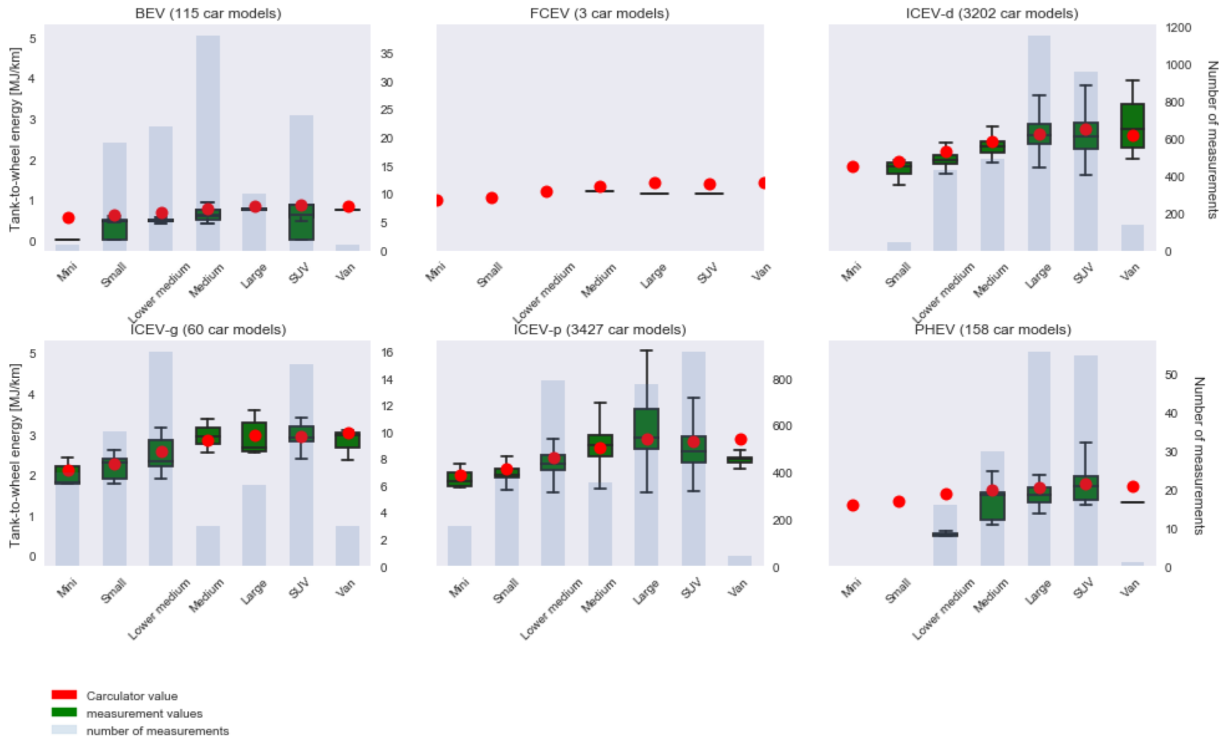


Figure 8 Validation of Tank-to-wheel energy requirement against the monitoring program for passenger vehicle emissions database. Horizontal lines within the green boxes represent the median value. The green boxes represent 50% of the distribution (25^{th}-75^{th} percentiles). The whiskers represent 90% of the distribution (5^{th}-95^{th} percentiles). Outliers are not shown. Source for vehicle tank-to-wheel energy consumption measurements: [57]

Once the calculated parameters values are obtained, the background part of the model consists into defining material and energy inventories and normalize them over a driving distance of one kilometer, before being characterized against midpoint environmental and economic indicators.

2.2 Vehicles background model

When all the material and energy attributes of the vehicle are defined, the required amounts of material and energy normalized over 1 kilometer are calculated.

2.2.1 Inventories for vehicle components

The model uses specific inventories from the literature for some of the vehicle components, initially detailed in [21]. Additional specific inventories relating to fuel pathways have been added and are listed in the Electronic Supplementary Information. *carculator* also sources less specific inventories from a time-adjusted version of the ecoinvent database version v3.6.

Specific inventories entail inventories for onboard energy storage (e.g., batteries of different chemistries, fuel tank for liquid and gaseous fuels), energy transformation (e.g., hydrogen-powered fuel cell stack) and fuel pathways (e.g., production and distribution of hydrogen, biogas, etc.). Inventories for the vehicle glider, the powertrain as well as the road infrastructures are sourced from the time-adjusted ecoinvent database.

2.2.2 Time-adjusted ecoinvent database

Using the Python library *rmnd-lca* [58], itself based on the *wurst* library [59], multiple time-adjusted versions of the ecoinvent database are produced. A similar endeavour had been realized before in the work of Mendoza Beltran et al. [44], where the ecoinvent database had been coupled to the integrated assessment model IMAGE [60], to modify life cycle datasets that relate to electricity generation. This time, multiple specific industrial sectors (e.g., electricity, heat, steel, cement) of the ecoinvent inventory database are adjusted to the energy scenario output of the integrated assessment model REMIND [48]. This includes, for example, the energy efficiency of power plants, the availability of secondary steel in the future, the share of biomass-derived and synthetic fuels in the conventional fuel blend, etc. Details on the coupling between ecoinvent and REMIND are available in the online documentation of the code repository. For the purpose of this study, the "SSP2-Baseline" and the "SSP2-PkBudg1100" energy scenario outputs of REMIND are used [61]. The "SSP2-Baseline" scenario lets the market regulate the development of energy technologies, without any specific climate policies enforeced, leading to an increase in the global temperature of more than 3.5 degrees Celsius by 2100. The "SSP2-PkBudg1100" scenario is target-driven, limiting the cumulative release of GHG emissions to 1,100 gigatons by 2100 (i.e., corresponding to an increase in the global temperature to well-below 2 degrees Celsius by 2100).

Additionally, emissions of non-greenhouse gases of power plants are aligned with the projections of the air emissions model GAINS [62]. *carculator* chooses inventories from the REMIND-based time-adjusted ecoinvent database that corresponds to the year of the vehicle production and the energy scenario defined by the user.

2.2.3 Electricity supply

The electricity supply mix used for charging the battery of BEV and PHEV, or producing hydrogen via electrolysis, can be selected from a list of over 80 countries. A user-defined electricity mix can also be specified. Current and future country-specific electricity supply mixes are available for each year between 2000 and 2050, based on energy projection models for the European Union [63], Africa [64], Switzerland – internal 2020 update from the STEM model [65] –, and other countries [66].

Unlike most LCA models of passenger vehicles, *carculator* uses an electricity supply mix which results from the uniform distribution of the annual kilometers driven over the years of use of the vehicle.

For example, should a BEV enter the fleet in Poland in 2020, most LCA models of passenger vehicles would use the electricity mix for Poland corresponding to that year, which corresponds to the row of the year 2020 in Table 3, based on the EU Reference scenario 2016 projection model [63]. *carculator* calculates instead the average electricity mix obtained from distributing the annual kilometers driven along the vehicle lifetime, assuming an equal number of kilometers is driven each year. Therefore, with a lifetime of 200,000 km and an annual mileage of 12,000 kilometers, the projected electricity mixes to consider between 2020 and 2035 for Poland are shown in Table 3. Using the kilometer-distributed average of the projected mixes between 2020 and 2035 results in the electricity mix presented in the last row of Table 3. The difference in terms of technology contribution and unitary GHG-intensity between the electricity mix of 2020 and the electricity mix based on the annual kilometer distribution is significant. The merit of this approach ultimately depends on whether the projections will be realized or not.

Table 3 Gross electricity production split by technology projected for Poland between 2020 and 2035, along with the unitary GHG-intensity, adapted from [67]

	Hydro	**Nuclear**	**Nat gas**	**Solar**	**Wind**	**Biomass**	**Coal**	**Oil**	**Geothermal**	**Waste**	**CO_2 intensity, at high voltage [kg CO_2-eq. per kWh]**
2020	1%	-	5%	-	6%	6%	82%	-	-	-	0.853
2021	1%	-	6%	-	7%	6%	80%	-	-	-	0.841
2022	1%	-	7%	-	8%	6%	77%	-	-	-	0.818
2023	1%	-	9%	-	9%	7%	75%	-	-	-	0.813
2024	1%	-	10%	-	10%	7%	72%	-	-	-	0.791
2025	1%	-	11%	-	11%	7%	70%	-	-	-	0.778
2026	1%	-	12%	-	11%	7%	69%	-	-	-	0.775
2027	1%	-	13%	-	11%	7%	68%	-	-	-	0.772
2028	1%	-	13%	-	11%	8%	67%	-	-	-	0.763
2029	1%	-	14%	-	11%	8%	66%	-	-	-	0.760
2030	1%	-	15%	-	11%	8%	65%	-	-	-	0.757
2031	1%	2%	16%	-	11%	8%	62%	-	-	-	0.735
2032	1%	4%	16%	-	12%	8%	59%	-	-	-	0.705
2033	1%	6%	17%	-	12%	9%	56%	-	-	-	0.684
2034	1%	8%	17%	-	13%	9%	53%	-	-	-	0.654
2035	1%	10%	18%	-	13%	9%	50%	-	-	-	0.632
Km-distributed	1%	1.8%	12%	-	10%	8%	67%	-	-	-	0.756

2.3 Life cycle impact assessment

To build the inventory of every vehicle, *carculator* populates a three-dimensional array A (i.e., a tensor) such as:

$$\mathrm{A} = [a_{ijk}], i = 1, \dots, L, j = 1, \dots, M, k = 1, \dots, N$$

The second and third dimensions (i.e., *M* and *N*) have the same length. They correspond to product and natural flow exchanges between supplying activities (i.e., *M*) and receiving activities (i.e., *N*). The first dimension (i.e., *L*) stores model iterations. Its length depends on whether the analysis is static or if an error propagation is performed (e.g., Monte Carlo).

Given a final demand vector *f* (e.g., 1 kilometer drive with a specific vehicle) of length equal to that of the second (or third) dimension of *A*, *carculator* calculates the scaling factor *s* using SciPy's linear solver for sparse matrices *spsolve* [68], so that:

$$s = \mathrm{A}^{-1} f$$

Finally, the scaling factor *s* is multiplied with a characterization matrix *B*. This matrix contains midpoint characterization factors for a number of impact assessment methods (as rows) for every activity in *A* (as columns). As described earlier, the tool chooses between several characterization matrices *B*, which contain pre-calculated values for activities for a given year, depending on the year of production of the vehicle as well as the REMIND energy scenario considered (i.e., "SSP2-Baseline" or "SSP2-PkBudg1100"). The midpoint indicators contained in the *B* matrix are listed in Table 4.

Table 4 Midpoint impact assessment indicators available in *carculator*

Midpoint indicator name	Unit	Method	Source
freshwater ecotoxicity	kg 1,4-DC.	ReCiPe Midpoint (H) V1.13	[69]
human toxicity	kg 1,4-DC.	ReCiPe Midpoint (H) V1.13	
marine ecotoxicity	kg 1,4-DB.	ReCiPe Midpoint (H) V1.13	
terrestrial ecotoxicity	kg 1,4-DC.	ReCiPe Midpoint (H) V1.13	
metal depletion	kg Fe-Eq	ReCiPe Midpoint (H) V1.13	
agricultural land occupation	square meter-year	ReCiPe Midpoint (H) V1.13	
climate change	kg CO_2-Eq	ReCiPe Midpoint (H) V1.13	
fossil depletion	kg oil-Eq	ReCiPe Midpoint (H) V1.13	
freshwater eutrophication	kg P-Eq	ReCiPe Midpoint (H) V1.13	
ionising radiation	kg U_{235}-Eq	ReCiPe Midpoint (H) V1.13	
marine eutrophication	kg N-Eq	ReCiPe Midpoint (H) V1.13	
natural land transformation	square meter	ReCiPe Midpoint (H) V1.13	
ozone depletion	kg CFC-11.	ReCiPe Midpoint (H) V1.13	
particulate matter formation	kg PM_{10}-Eq	ReCiPe Midpoint (H) V1.13	
photochemical oxidant formation	kg NMVOC-.	ReCiPe Midpoint (H) V1.13	
terrestrial acidification	kg SO_2-Eq	ReCiPe Midpoint (H) V1.13	
urban land occupation	square meter-year	ReCiPe Midpoint (H) V1.13	

water depletion	m^3 water	ReCiPe Midpoint (H) V1.13	
human noise impacts	person.Pascal.second	Human noise impacts	[53,70]

Additionally, it is possible to export the inventories in a format compatible with the LCA framework Brightway2 [45], thereby allowing the characterization of the results against a larger number of impact assessment methods.

2.4 Comparative analysis in European countries

For this case study, the scope of analysis is limited to gasoline-powered ICEV and BEV of a lower-medium size for the 27 Member States of the European Union, in addition to the United Kingdom, Norway and Switzerland. For each country, the corresponding time-distributed electricity mix is used. The comparative analysis for each country is performed considering error propagation (Monte Carlo analysis) from the input parameters over 1,000 iterations. The error propagation analysis is run twice, using each of the two energy scenarios of the REMIND model in the background inventory database – namely “SSP2-Baseline” and “SSP2-PkBudg1100”. Also, this analysis does not consider the expected progression of 2nd generation biofuels in the gasoline blend in Europe. Finally, it is important to note that ICEV undergo a mild hybridization of their powertrain over time, where up to 18% of the required power is provided by an electric engine by 2050. Results are represented as a minimum-maximum interval. Its boundaries are calculated as the 25th percentile of the Monte Carlo distribution using the “SSP2-PkBudg1100” energy scenario as a minimum, and the 75th percentile of the Monte Carlo distribution using the “SSP2-Baseline” energy scenario as a maximum. While such definition of boundaries is unusual, it allows to consider the amplitude of possible results associated to the future global energy policy, combined with the uncertainty of the foreground vehicle model itself.

The next section describes the results of the comparative analysis and presents a few parameters end-results may be sensitive to.

3 Results

Figure 9 shows the results of the comparative error propagation analysis between a BEV and an ICEV-p of a lower-medium size class. The life cycle inventories used to produce these results for the year 2020 are detailed in the Electronic Supplementary Information. In all countries but Estonia and Poland, starting to drive a BEV in 2020 provides benefits in regard to GHG emissions over the lifetime of the vehicle. The decrease in GHG emissions for gasoline-powered ICEV over time is explained by material and energy efficiency on one hand, and a progressive hybridization of the powertrain on the other hand. ICEV-p become more fuel-efficient thanks to a decrease in the curb mass of the vehicle by 8.5% between 2020 and 2050, and a parallel relative increase of the powertrain and engine efficiency of 50% in that same period, resulting in a reduction of the tank-to-wheel energy consumption by almost 48% -- 2.3 MJ/km in 2020, against 1.2 MJ/km in 2050. In that same period, the share of the power output provided by an internal combustion engine goes from 100% to 85%, allowing to downsize the combustion engine and operate it more often at full power, thereby increasing the efficiency of the powertrain. This brings the fuel efficiency-related exhaust emissions from 180 g CO_2-eq./km in 2020 down to only 91 g CO_2-eq./km in 2050. The results for ICEV-p are largely insensitive to the location. Life-cycle GHG emissions for BEV are, in contrast to ICEV, more sensitive to the location of use. They have generally lower emission levels compared to ICEV-p throughout the period considered. Their tank-to-wheel energy consumption is initially lower in 2020, thanks to a more efficient powertrain. But the latter, being already high, does not improve much in the future and cannot solely explain the drop of 25% of the tank-to-wheel energy consumption. Instead, the decrease in the curb mass by 12% and improved heating and cooling systems contribute to reducing energy consumption. This is combined with a reduction of the emissions associated to the production of electricity in most countries. It results, on average across the countries considered, in a decrease of the energy chain-related emissions of 60%, going from 80 g CO_2-eq./km in 2020, down to 35 g in 2050. In parallel, non energy chain-related emissions, largely represented by the production of the glider and the powertrain, have decreased by 30% only. Interestingly, in countries like Malta and Luxembourg, ICEV-p become the preferred option after 2035, as efforts in increasing the powertrain efficiency may outpace efforts in decarbonizing the national electricity grid.

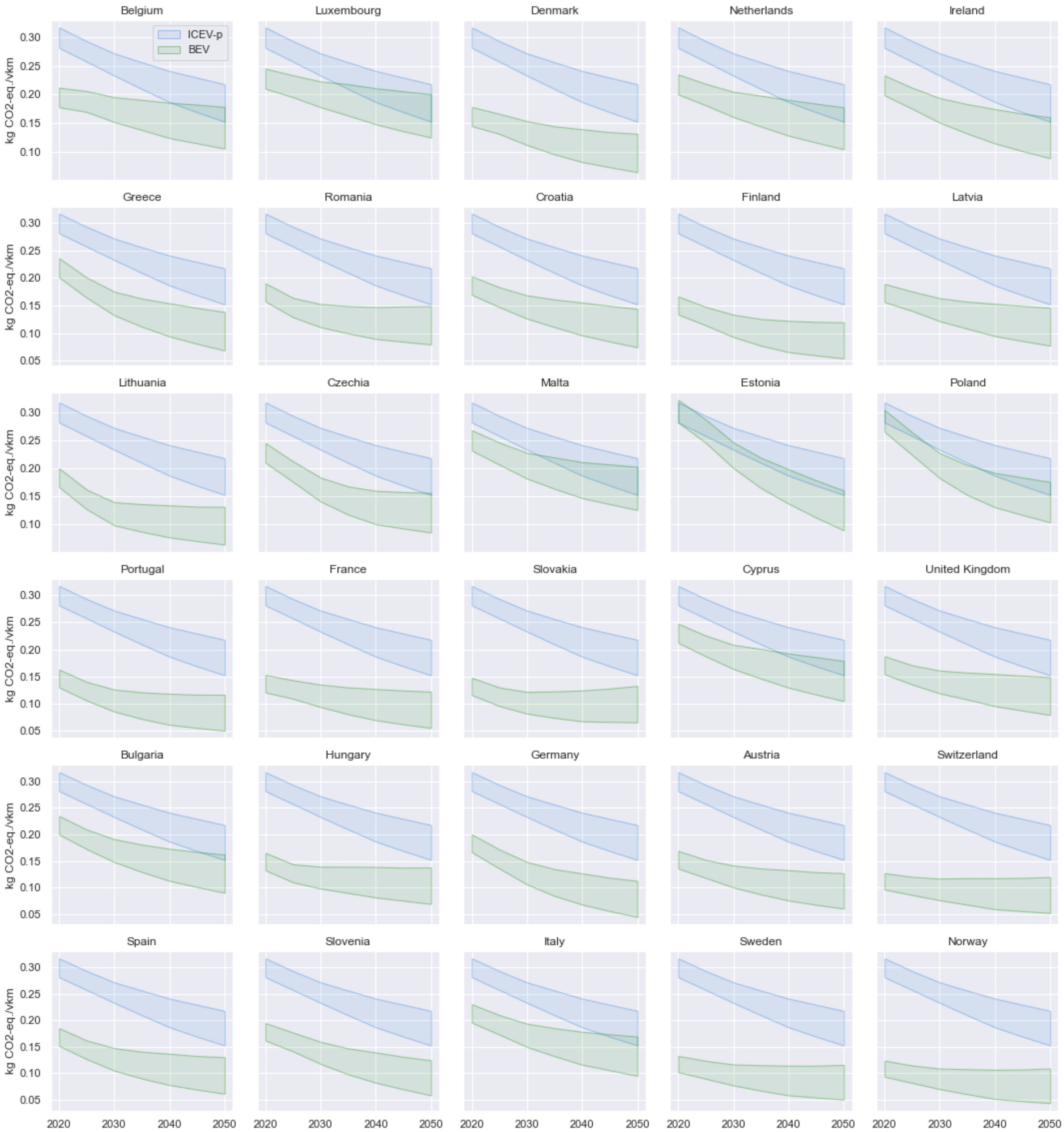


Figure 9 Life cycle GHG emissions of ICEV-p and BEV in EU-27, Norway, Switzerland and the United Kingdom, including error propagation analysis. Lower interval boundary: 25^{th} percentile of Monte Carlo distribution using the "SSP2-PkBudg1100" REMIND energy scenario in the background inventory database. Upper interval boundary: 75^{th} percentile of Monte Carlo distribution using the "SSP2-Baseline" REMIND energy scenario in the background inventory database.

3.1 Sensitivity analysis

This section briefly describes the model parameters that can influence the results presented previously most substantially.

3.1.1 Electricity supply mix

Life cycle assessment results are sensitive to a few calculated parameters. For BEV, the carbon intensity of the electricity supply mix is an important one. Figure 10 depicts the effect of the carbon intensity of the electricity mix used for battery charging on the potential climate change impacts of a BEV of a lower-medium size class, compared to that of a gasoline-powered vehicle (ICEV-p), in 2020, 2030, 2040 and 2050. The figure shows that the potential climate change impacts of a BEV reduce dramatically for each additional percent of electricity share provided by solar panels, at the expense of coal-based electricity. This translates into an electricity supply mix with a lower carbon intensity, as shown in the secondary x axis of the graph. The same holds true for any other type of renewable energy source with similarly low GHG emissions. In 2020, the intersection between the BEV and ICEV-p slopes indicates that a minimum contribution of solar power of 20% -- or a maximum coal-based power contribution of 80% --, is required for BEV to perform better than ICEV-p in regard to potential climate change impacts, on the basis of one kilometer driven. This corresponds to a carbon intensity of the electricity mix of approximately 800 g. CO_2-eq./kWh. For other years, the threshold to reach for levels of solar power integration in the electricity supply mix is higher: at 30%, 40% and 50% for 2030, 2040 and 2050, respectively. This is because *carculator* projects that ICEV-p profit from an increased efficiency of the powertrain due to a mild hybridization in the future, allowing for the partial recuperation of braking energy.

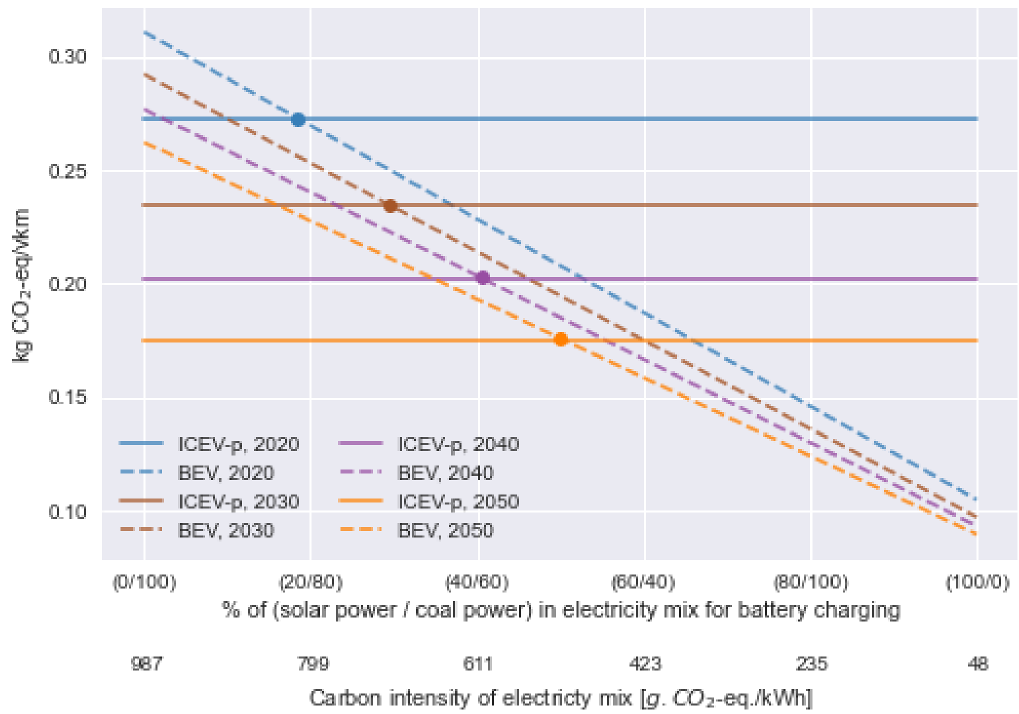


Figure 10 Effect of increasing the share of solar power at the expense of coal-based power in the electricity mix used for battery charging on the GHG emissions of a medium-size BEV

3.1.2 Other vehicle parameters

End-results may also be sensitive to other vehicle parameters. *carculator* offers a convenient function to perform "one-at-a-time" sensitivity analyses on all vehicles. By default, the tool increases each input parameter by 10% individually and measures the changes within the end-results. Such analysis is performed for lower-medium BEV and ICEV-p vehicles with the production year of 2020, with respect to the potential Global Warming impacts (GWP). The results are illustrated in Figure 11 and Figure 12, for ICEV-p and BEV respectively. For ICEV-p, increasing the engine or drivetrain efficiency would decrease end-results in terms of GWP by a factor of over 1.06. Inversely, increasing the mass of the glider, the aerodynamic drag, or the frontal area of the vehicle would increase said end-results by a factor of 1.02 to 1.05. Regarding BEV, the charge and discharge efficiencies of the battery can reduce GWP results by a factor of 1.04-1.06. The engine and drivetrain efficiencies and the expected kilometric lifetime are also parameters that can "positively" impact GWP results. On the other hand, GWP results are "negatively" impacted following positive value changes for the glider mass, the aerodynamic drag coefficient, the frontal area of the vehicle, the rolling resistance and the mass of the battery.

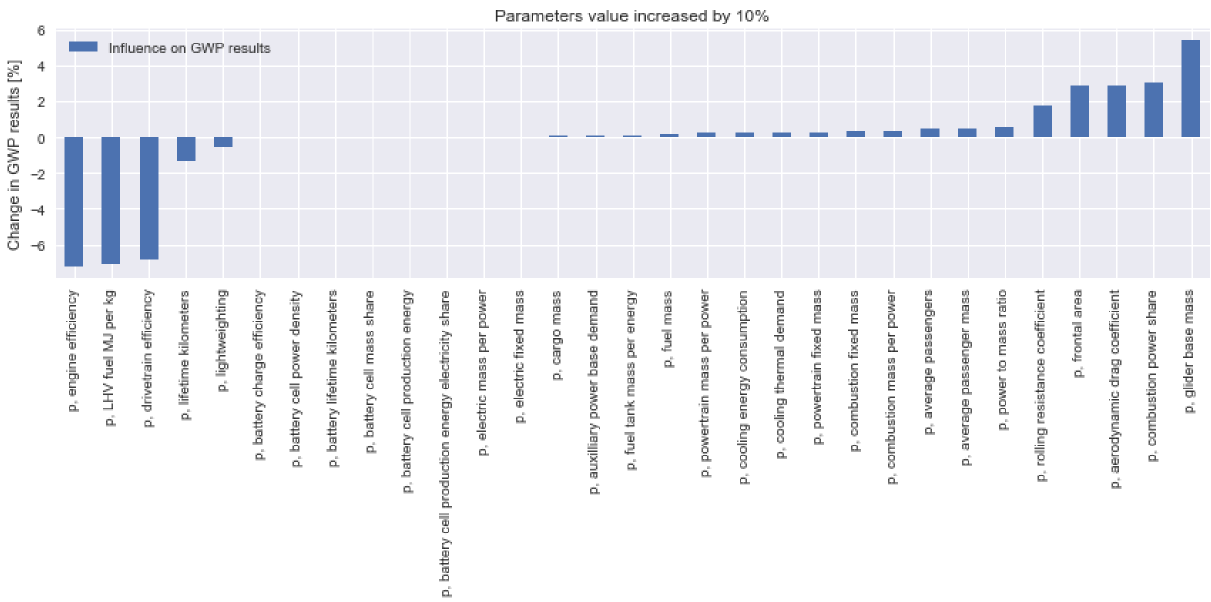


Figure 11 Sensitivity of GWP results in regard to parameters for ICEV-p

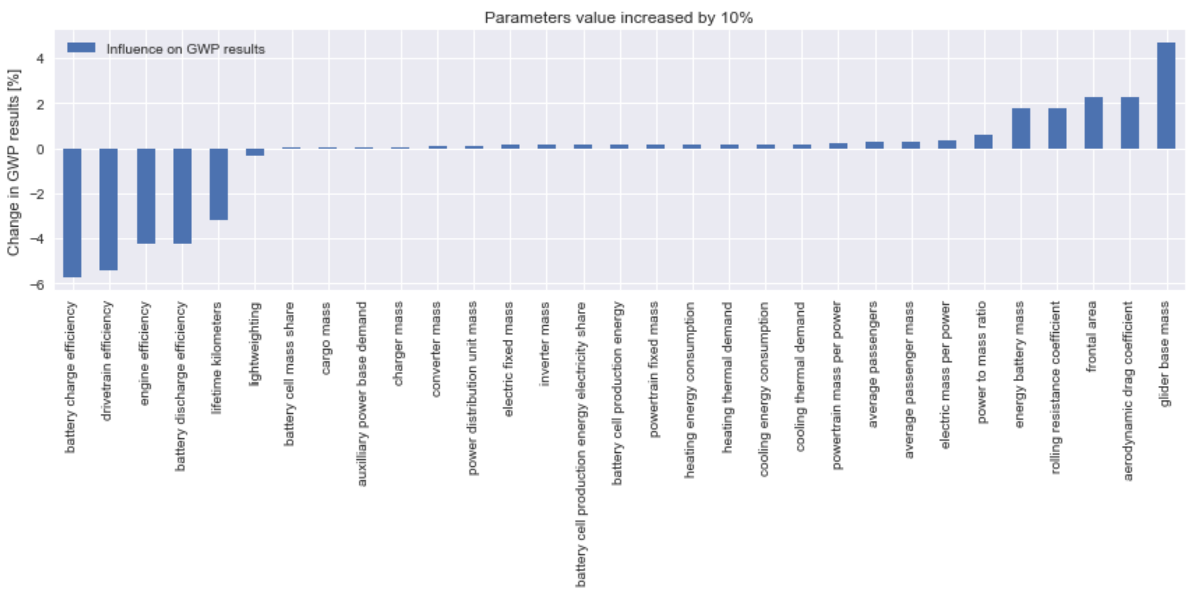


Figure 12 Sensitivity of GWP results in regard to parameters for BEV

4 Discussion

The section discusses a few aspects of the tool: what its limitations are, how it will be improved and its online graphical user interface.

4.1 Limitations

This tool provides a robust framework in terms of model transparency and comprehensiveness. Yet, as with all models, it is not free of limitations. A first limitation is that *carculator* quantifies life-cycle environmental burdens (and costs) of generic vehicles of specific size-categories, but not of single vehicle models. However, the analysis of a specific model is possible, provided that input parameters specific to the vehicle model are known and default values adjusted accordingly.

A second limitation lies in the fact that the tool does not easily allow to model specific supply chains. While it is possible to choose the origin of manufacture for Li-ion batteries – which determines the sources of electricity and heat for the production of battery cells, for example –, it is not yet possible to adjust the transportation mode and distance to supply the said battery to the location of assembly.

Also, the tool uses average exhaust emission factors according to HBFA 4.1 [71]. These emission factors might underestimate emissions on road of specific vehicle models not complying with emission standards under all circumstances [72].

Moreover, toxicity-related impacts depend on the location of emissions of specific pollutants. While the current version of the tool is able to discern different emission compartments for exhaust emissions based on speed levels during the driving cycle, it does not have such geographical resolution for emissions that occur during the production phase of the vehicle and its components. This may impede the accuracy of the model, especially in regard to the extraction and refining of rare earths and other metals required for the battery and onboard electronics, for example.

The inventory data used for the production of the vehicle glider also represent a limitation as they are relatively old (i.e. early 2000's) and are therefore unlikely to represent modern vehicles very well, especially regarding electronics. This should, however, not have a major impact on potential climate change impacts. Other impact categories might be affected to a larger extent.

Finally, it is worth noting that the national electricity consumption mixes used for battery charging in this study are not marginal, but average. They reflect adequately the nature and composition of the electricity used for the operation of a single car, given a penetration rate for BEV defined by the energy scenario used to produce these electricity mixes. But such electricity mixes would look different considering a sinigificant increase in demand for electricity, as a result of a higher-than-expected penetration rate of BEV. This can potentially change the conclusion of this study. However, this limitation is not inherent to the tool, but rather to its data input.

4.2 Outlook

The framework of the tool will be extended in different directions. More precisely, the vehicle portfolio will be extended. In addition to passenger vehicles, other means of transport will be added, such as planes, trains, trucks, buses, motorcycles and bicycles. This will allow to compare the environmental burdens of different options, including public transport using a passenger-kilometer basis, but also freight hauling, based on a ton-kilometer.

In regard to onboard energy storage, additional battery types will be added, on top of the three types of Li-ion battery chemistries currently available to equip battery electric and plugin hybrid vehicles (i.e., NMC, NCA and LFP). Also, the tool will offer the option to perform consequential LCA to quantify the environmental impacts associated to an increase in demand for a particular type of vehicle. This is expected to show differences on how the supply of electricity, heat and steel are modeled, among others. For the supply of electricity, the tool will include the respective country-specific long-term marginal electricity mixes provided by Vandepaer et al. [73]. Finally, key inventory data will be kept up-to-date, both in the foreground model (e.g., exhaust emissions, fuel cell and battery inventories) and in the background model, achieved by a deeper coupling between newer versions of ecoinvent and integrated assessment models, such as REMIND, IMAGE or TIMES-based energy models like STEM [65].

4.3 Online graphical user interface

Developing a transparent tool that allows to reproduce LCA results for passenger vehicles is a substantial step forward in this area of research. Yet, the tool requires knowledge of the Python programming language, which is not within everyone's reach. Therefore, an online graphical user interface has been developed. It can be accessed at https://carculator.psi.ch and used by anyone in order to answer specific research questions, investigate the impact of certain boundary conditions as well as different future scenarios. It aims at eliminating wrong beliefs, contributing to a fact-based discussion and ideally leading to an informed decision-making process.

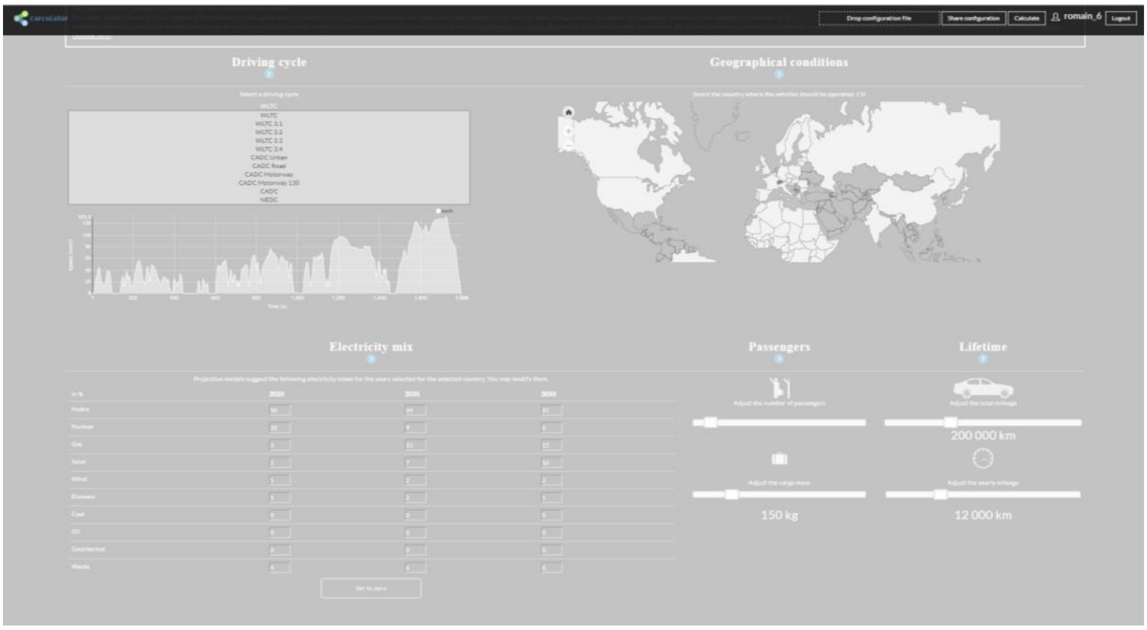


Figure 13 Screen capture of the online graphical user interface

4.4 The case study

The case study shows that BEV cause lower life-cycle GHG emissions than gasoline ICEV in most European countries, using time-distributed country-specific power supply mixes for battery charging. GHG emissions reduction caused by switching from ICEV to BEV is substantial in countries with large shares of renewable energy or nuclear power. This would be the case in France, Iceland, Norway, Sweden and Switzerland. In the case of Poland and Estonia, two countries with a large share of electricity supplied by coal-fired power plants, operating a BEV does not lead to a reduction of GHG emissions for the time being. However, the situation is expected to change in 5 to 10 years time, if decarbonization goals would be reached. This prospective analysis shows that benefits associated to the electrification of powertrains are expected to increase. This is due to two main dynamics. On one side, there is the expected progress in the automotive sector in terms of material and energy efficiency. On the other side, the European decarbonization goals push forward the deployment of renewable energy sources, at the expense of fossil-based technologies. Notwithstanding a great potential for GHG emissions reduction, replacing ICEV with BEV will not be sufficient to reach the EU's "zero-emission" for the transport of passengers. Indeed, the GHG emissions associated with the vehicle production can only be eliminated if the energy supply world-wide would refrain from using fossil fuels. This stresses the importance of embodied GHG emissions in imported goods and services. Alternatives to individual transport must therefore be expanded and become more attractive.

5 Conclusion

The primary goal of this article is to introduce *carculator*, an open-source Python library to assess the life cycle emissions and cost of passenger vehicles. A case study is presented to examplify the flexibility and convenience of the tool. With a few lines of code, *carculator* compared the projected evolution of GHG emissions for battery electric and gasoline-powered vehicles. To do so, it uses country-specific time-distributed electricity mixes. Results show that in 28 out of the 30 countries considered, operating a battery electric vehicle in 2020 will reduce GHG emissions compared to a gasoline-powered vehicle over its lifetime. Despite a significant potential for decreasing GHG emissions at the *use* phase through the decarbonization of electricity mixes combined with an expected increase in material and energy efficiency in the automotive sector, embodied GHG emissions at the *production* phase will persist.

Software and data availability

- Name of software: carculator
- Version: 1.0.0
- Developers: Romain Sacchi, Christopher Mutel, Brian Cox
- Online repository: https://github.com/romainsacchi/carculator
- Documentation: https://readthedocs.org/projects/carculator/
- Online graphical user interface: https://carculator.psi.ch/
- Contact information: carculator@psi.ch
- Year first available: 2020
- Software required: Python 3.7
- Availability: Open source
- Cost: Free
- Program language: Python
- Program size: 38 megabytes
- Archive: https://zenodo.org/record/3778259#.Xqqpq8j7R3g
- DOI: 10.5281/zenodo.3778259
- Size of archive: 1,900 kilobytes

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