# Environmental assessment of road transport based on ammonia from a life cycle perspective

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## 1 Abstract

Several alternatives at different development stages are being considered to achieve the transport sector's decarbonisation goals. Ammonia has the potential to be a viable option, and it is critical to study its environmental profile in this early phase to appraise its sustainability as a fuel for private transportation. This work aimed to develop a life cycle assessment, from the cradle to the grave, of an ammonia-fuelled internal combustion engine passenger car, considering the effect of different operation modes and vehicle emission control strategies, which resulted in nine configurations. Using of Fe and Cu-exchanged zeolites as catalysts in the after-treatment system showed the best environmental profile in four of the six categories evaluated, including climate change. While, for photochemical oxidant formation and terrestrial acidification, the optimum control strategy is using a fuel equivalence ratio of 1.1. On average, per 1 km travelled in an ammonia-based ICE passenger car represents 0.098 kg $CO_2$-eq for global warming potential (GWP100), 30.755 g oil-eq for fossil depletion potential (FDP), 38.974 mg P-eq for freshwater eutrophication potential (FEP), 8.907 µg CFC-11-eq for ozone depletion potential (ODP), 0.906 g NMVOC-eq for photochemical oxidant formation potential (POFP), and 1.029 g $SO_2$-eq for terrestrial acidification potential (TAP100). These results show a significant reduction, above -70%, for GWP100, FDP, and ODP, compared with the same vehicle fuelled on gasoline.

## 2 Keywords

ICE, transport, LCA, ammonia, hydrogen, energy, decarbonisation, vehicle

## 3 Introduction

Ammonia has been fully recognised as a chemical with the potential to deliver green hydrogen over long distances and for heavy loads [1–4]. Since 2018, the International Energy Agency (IEA) has realised the considerable potential of using a well-traded commodity to store and flexibly distribute energy obtained from renewable sources such as wind, solar, and marine [5]. However, several challenges still remain for using ammonia as a fuelling vector. Out of all the main challenges recognised in the transition to a hydrogen-ammonia economy [6], public perception, adequate legislation and better knowledge of environmental impacts are probably the most complex to deal with. The vast trade-offs from the use of ammonia and the effects the chemical could possess, make imperative comparative life cycle assessments capable of providing further guidance for decision-making processes.

Life Cycle Assessment (LCA) is a methodology that helps researchers and practitioners quantify the potential impacts of a good or a service throughout its entire life cycle. LCA has been used extensively for private road transport [7], and a few have been developed over the years to use ammonia as a fuelling vector. Angeles et al. [8] compared the nitrogen and carbon footprint of various fuels assessed whilst employed in propulsion systems (i.e. fuel cells and internal combustion engines). Ammonia and ammonia/gasoline blends were studied, and it was found that fuel cell vehicles fed with ammonia would produce the lowest environmental footprint. Separately, Angeles et al. [9] found that using a blend of biomass-based ammonia and gasoline, internal combustion engine vehicles could deliver lower carbon footprint profiles than diesel or gasoline.

Similarly, Bicer and Dincer [10] analysed various city transportation and power generation systems fuelled with ammonia from nuclear plants. The results denoted a considerable decrease in greenhouse gas emissions with an acute impact on global warming potential. However, the results also demonstrated that with the reduction of carbon footprint, the increase in nitrogen-based species (i.e. NOx and $N_2O$) could be considerably high, shadowing the overall balance in greenhouse gas mitigation, as recently shown in [11] for single cylinder engines. The emissions profile during vehicle operation used in this study were extrapolated; no actual vehicle operation data could be founded. This study includes four impact categories (Abiotic depletion, Acidification, Global warming, and Ozone layer depletion). Interestingly, further results [12,13] show ammonia's impact on various transportation methods. In vehicles, the reduction of greenhouse gases (GHG) can be considerable [14], with values that go from 0.270 to 0.100 kg CO2-eq/km transported, whilst in power plants, the combustion process carbon footprint (which generated up to 97% GHG of the entire cycle) can be substantially mitigated (to 6%) by using ammonia [10].

A more recent study by Razon and Valera-Medina [15] shows how using wind turbines or nuclear power to produce ammonia fuelling for power gas turbines can drastically reduce the global warming potential of these units. Employing electrolysis, green hydrogen was used for the production of ammonia. Under these scenarios, a reduction of 28 to 32% global warming potential was observed compared to a methane-based case. Interestingly, the two environmental impacts linked to the emission of nitrogen oxides, aquatic acidification and terrestrial acidification/nitrification, decrease as the fuel equivalence ratio increases. As the fuel equivalence ratio exceeds 1.2, these parameters become lower than the referred methane value [15]. It is important to emphasise that current efforts are based on developing rich ammonia combustion regimes close to a 1.2 equivalence ratio for gas turbines, a concept still under research for internal combustion engines [16].

Further LCA analyses were performed by Boero et al. [17], who studied a gas turbine power cycle [18] fed with ammonia/hydrogen under humidified conditions. Mashruk et al. [19] showed efficiencies ~60%, whilst the LCA study demonstrated that using heat and power with the implementation of ammonia-based engines could provide both efficient power production and positive environmental impacts. Cradle-to-gate assessments showed how renewable and nuclear energy employed for water electrolysis gives better profiles regarding global warming, fossil depletion, and ozone depletion potential. Several scenarios were assessed (i.e., Morocco, Australia, Chile, Brazil, Iceland and the United Arab Emirates, and the United Kingdom; this last one with and without carbon capture and storage), each showing high carbon footprints when renewable ammonia was not employed. However, using renewable or nuclear sources ensured drastic reductions (i.e. -41% without co-generation and wind energy) in the global warming potential of these technologies. Carbon capture and storage were also found to help reduce environmental impacts, but not as much as initially conceived. Finally, it is also calculated that greater efficiencies in the production of ammonia (i.e. Haber-Bosch process) could also reduce the environmental impact of using ammonia as a fuelling vector.

Recent studies [20] have also compared various energy carriers, namely liquefied natural gas, methanol, DME, liquid hydrogen and liquid ammonia from renewable and conventional sources. The analyses include all the life cycles of these carriers from production, storage, and transport (20,000 nmi) to utilisation in an internal combustion engine. It was found that when natural gas is used in the production process, liquid ammonia is the most polluting fuel. However, liquid hydrogen becomes the cleanest solution, followed by ammonia if solar energy is employed in hydrogen production. Although there is a reduction in $CO_2$ with methanol and DME, their values are higher than those produced from liquified natural gas. Hence, the analysis emphasises the importance of producing green hydrogen or ammonia for decarbonising [20]. It is worth noticing that the emissions profile during the operation of this study does not include pollutants such as dinitrogen oxide ($N_2O$) present in the ammonia combustion process.

A recent report produced by the Maritime Cleantech Cluster [21] showed that using liquid ammonia in internal combustion engines for maritime purposes can lead to “net zero carbon emissions” in the combustion chamber. However, careful considerations need to be taken to avoid large GHG emissions during the production of the molecule itself, whilst further analyses of other emissions still require investigation. As previously depicted, if ammonia is employed using fossil fuels without CCS (grey ammonia), the carbon footprint impact is much higher than using these fossil fuels directly into the thermodynamic cycle. The report also raises the importance of thoroughly evaluating some of the most environmentally damaging molecules of ammonia combustion, $N_2O$, which requires further studies. Thus, it was concluded that ammonia is not a “zero-emissions” combustion fuel, and the amount of GHG is highly dependent on the ammonia production pathway. A similar conclusion was drawn by Mallouppas et al. [22] in their review of the latest advances in using ammonia as an alternative fuel in the maritime industry. They emphasised the need to study the whole lifecycle of ammonia to assess its global warming potential. They also advocated that more research must develop (simulations and experimental testing) to derive strategies to enhance the combustion of ammonia.

In this regard, the latest research on ammonia as fuel in internal combustion engines has focused more on compression ignition (CI) than spark-ignition (SI) engines [23] because of the greater installed capacity of the former and, consequently, their applications in transportation and power generation [24,25]. Nevertheless, in various studies [23,26–30], researchers have demonstrated the suitability of ammonia as fuel in SI engines, considering different operating conditions to improve combustion stability and efficiency and reduce pollutant nitrogen compounds emissions.

To the authors’ knowledge, no previous LCA study has included an operation emissions profile focusing on nitrogen compound emissions to evaluate the environmental impact of vehicles operating on ammonia solely. Therefore, the aims of this work are to (i) model an emissions profile of ICE vehicles operating on ammonia, considering the effect of the different operation modes and nitrogen emission control strategies, (ii) evaluate the environmental profile of ammonia as an alternative fuel for internal combustion engine vehicles from a life cycle perspective, and (iii) compare the environmental profile of ammonia-based ICE with the Euro 6 standard for gasoline and diesel.

# 4 Methods

## 4.1 Life Cycle Assessment

This LCA has been developed following the ISO framework, 14040 and 14044 [31,32]. The scope of this work constitutes a cradle-to-grave approach for the system shown in Figure 1, considering 1 km travelled as the Functional Unit, FU.

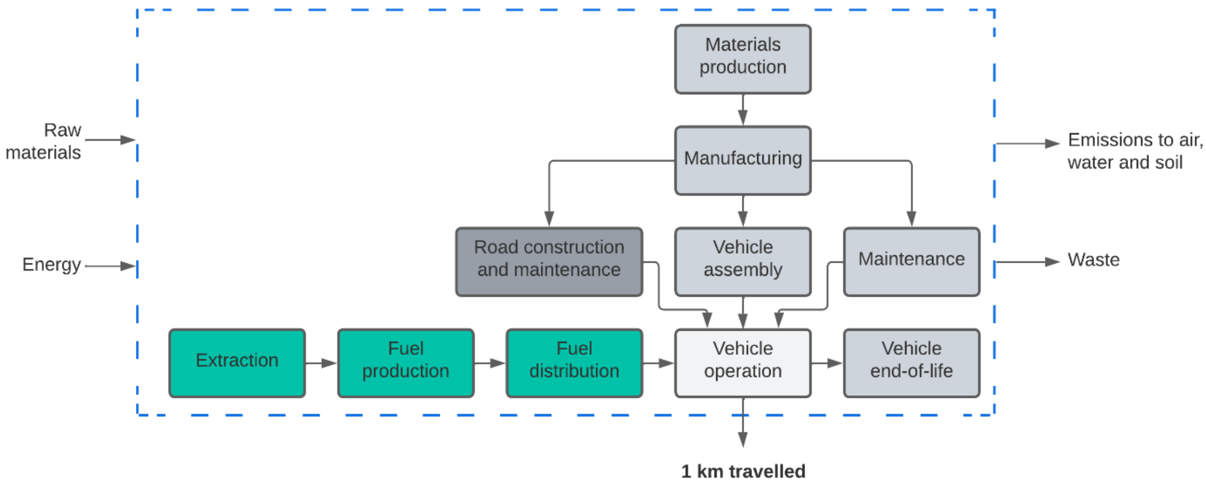



*Figure 1: System Boundaries for the LCA of an ammonia-fuelled ICE passenger car*

The Life Cycle Inventory (LCI) is the systematic compilation of inflows and outflows associated with the system during its life cycle. In this study, the LCI can be grouped as (i) vehicle (manufacturing, operation and maintenance, and end-of-life), (ii) infrastructure (road construction and maintenance), and (iii) energy production (extraction, processing, and distribution of the fuel, ammonia in this case). The LCI was compiled both with background and primary data.

The study considers using green ammonia from renewable energy (wind) produced in the UK. The ammonia production processes inventory was obtained from Boero et al. [17], while the vehicle manufacturing, maintenance, and infrastructure processes, were from the Ecoinvent 3.7.1 database [33]. The operation of the ammonia-based vehicle, fuel consumption and air emissions constitute primary data derived from the results of the model described in subsection 2.2 Vehicle and engine model. For the comparison with Euro 6 standard, fuel consumption and air emissions of gasoline and diesel ICE vehicles were obtained from Sisani et al. [34].

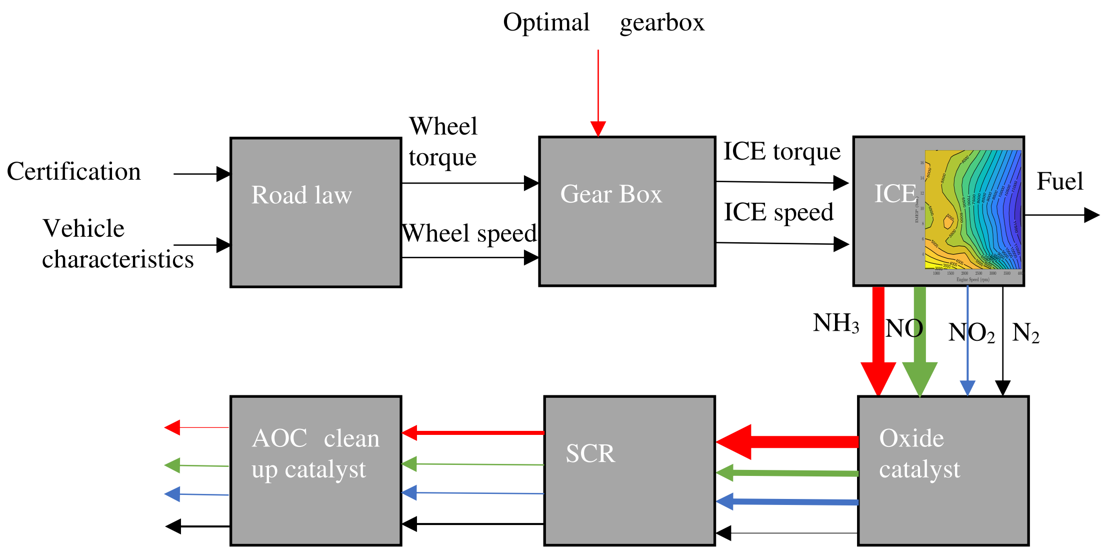
The final steps of an LCA are life cycle impact assessment (LCIA) and interpretation. In the LCIA, the potential impacts are estimated based on the LCI by implementing ReCiPe2016 Midpoint (H) v1.13 methodology. The included impact category indicators are global warming potential (GWP100, kg $CO_2$-eq, also known as carbon footprint), fossil depletion potential (FDP, kg oil-eq), freshwater eutrophication potential (FEP, kg P-eq), ozone depletion potential (ODPinf, kg CFC-11-eq), photochemical oxidant formation potential (POFP, kg NMVOC-eq), and terrestrial acidification potential (TAP100, kg $SO_2$-eq). The software used to perform the calculations was OpenLCA [35].

## 4.2 Vehicle and Engine modelling

The vehicle chosen for the simulation was a B-segment type vehicle fuelled with neat ammonia, with characteristics shown in Table 1. The global scheme of the model, presented in Figure 2, is decomposed into several sub-models. First, depending on the homologation cycle (WLTC or NEDC) and vehicle characteristics, one can model the force needed by the vehicle to run at the speed defined by the cycle. To do so, the torque at the wheel, $T_{wheel}$, is defined to balance equation Eq.1. An algorithm determines the gearbox ratio to minimise the polluting emissions or the fuel consumption. The gearbox ratio will then define the torque and engine speed necessary to move the vehicle forward, as long as the requested values are within the load/engine speed range provided by the thermal engine, as indicated by the Internal Combustion Engine (ICE) map.

$$F_{rolling} = T_{wheel} * R_{wheel} = F_0 * m_{veh} + F1 * V_{veh} + F2 * V_{veh}^2 + m_{veh} * \frac{dV_{veh}}{dt} \qquad (Eq. 1)$$

The fuel consumption and the exhaust pollutant emissions were estimated from previous single-cylinder engine tests obtained with the engine (characteristics shown in Table 3), and some engine performance results can be found in [30]. As a function of the wheel torque, the vehicle speed and the gearbox ratio, the operating point can move within the ICE map, thus giving fuel consumption and pollutant emissions for each time step.




$$2NO + 2NO_2 + 4NH_3 \rightarrow 4N_2 + 6H_2O$$

*Figure 2: scheme of vehicle model*

*Table 1: Modelled vehicle characteristics*

| | |
|---|---|
| Vehicle Weight | 1800 kg |
| Gear box ratios | 0.5; 0.84; 1.18; 1.52; 1.86; 2.2 |
| Axle ratio | 3.882 |
| F0 | 0.1 N/kg |
| F1 | 0.5 N/(km/h) |
| F2 | 0.03 N/(km/h) ² |

*Table 2: Modelled engine characteristics*

| | |
|---|---|
| Engine Displacement | 1.6 L |
| Compression Ratio | 10.75 |
| Max Torque | 260 Nm |
| Max Power | 95 kW |

In this model, several assumptions were imposed, namely: i) as the engine mapping was performed in steady-state conditions, the model does not consider the eventual increase in emissions related to transient operations. ii) the engine was running in stable, warmed conditions; therefore, the impact of engine warm-up at the beginning of the cycle on fuel consumption and polluting emissions was not modelled.

***Parameters variation***
The ICE map was modelled as a function of equivalence ratio (ϕ) and Exhaust Gas Recirculation rate (EGR) and as they impact NOx and $NH_3$ emission levels. However, in the framework of this study, the change of ϕ and EGR rate during the cycle was not modelled; therefore, EGR rate and equivalence ratio values must be defined before running the cycle and kept constant during the whole simulation.

***After-treatment system modelling***
Concerning the after-treatment system, since no dedicated after-treatment system exists for neat ammonia combustion up to now, several assumptions were made. Firstly, an oxide catalyst model was considered in order to have similar volume amounts of NO and $NO_2$ at the input of the Selective Catalyst Reduction (SCR) after-treatment system, to favour the reaction indicated in Equation 2. Secondly, the SCR system was modelled according to three main families of catalysts, namely the V-based catalysts ($V_2O_5$, $WO_3$, $TiO_2$), the Fe-exchanged zeolites and Cu-exchanged zeolites, as presented in [36]. The main differences between these technologies are the efficiency curve as a function of the exhaust temperature and the amounts of $NH_3$ slipped and $N_2O$ formed (Figure 3). In the present study, $NH_3$, $NO_x$ and $O_2$ storage during transients are not modelled. In fact, for each time step, the conversion of $NO_x$ and $NH_3$ as well as the amount of ammonia slipped, are computed depending on both exhaust temperature and [$NH_3$/$NO_x$] ratio, shown in Figure 3.a. Therefore, no addition of $NH_3$ is considered to ensure an $NH_3$/$NO_x$ optimal ratio. The effect of the SCR technology on the conversion efficiency and $NH_3$ and $N_2O$ slip, as a function of the exhaust temperature, is shown in Figure 3.b.

$$2\,NO + 2NO_2 + 4NH_3 \rightarrow 4N_2 + 6H_2O \qquad (Eq.2)$$

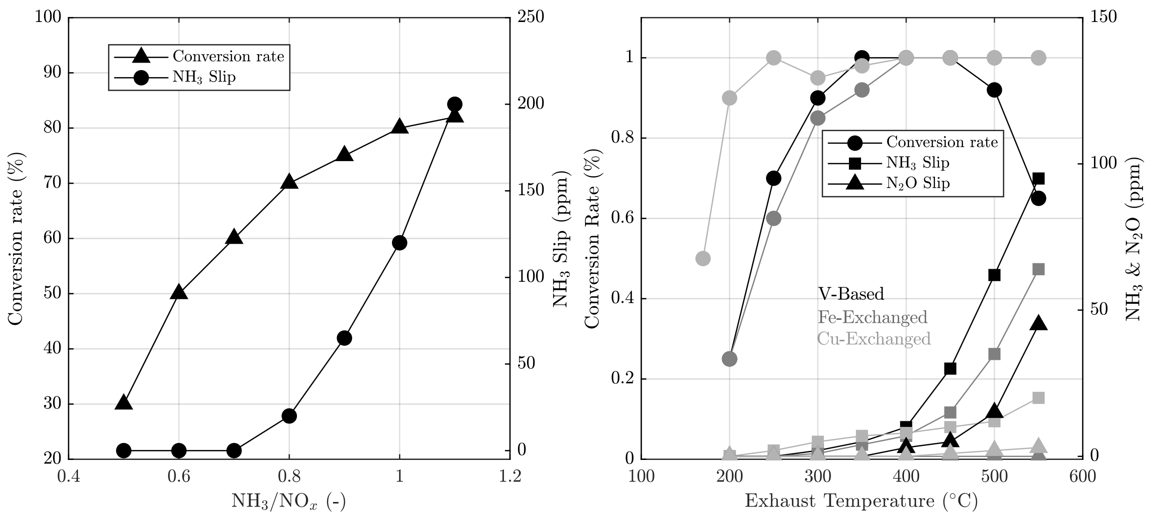



*Figure 3: a) SCR conversion rate and ammonia slip as a function of NH3/NOx ratio. b) SCR conversion rate and ammonia slip depending on both SCR technology and exhaust temperature* [30].

Table 3 summarises the nine model configurations included in the study.

*Table 3: Vehicle and engine model configurations*

| **Parameters** | **Equivalence ratio** | **EGR rate** | **Gearbox optimisation criterion** | **After treatment system** |
|---|---|---|---|---|
| Configuration 01 | 1 | 0 | $NO_x$ | V-Based |
| Configuration 02 | 0.9 | 0 | $NO_x$ | V-Based |
| Configuration 03 | 1.1 | 0 | $NO_x$ | V-Based |
| Configuration 04 | 1 | 5 | $NO_x$ | V-Based |

| **Parameters** | **Equivalence ratio** | **EGR rate** | **Gearbox optimisation criterion** | **After treatment system** |
|---|---|---|---|---|
| Configuration 05 | 1 | 10 | $NO_x$ | V-Based |
| Configuration 06 | 1 | 0 | $NO_x$ | Fe |
| Configuration 07 | 1 | 0 | $NO_x$ | Cu |
| Configuration 08 | 1 | 0 | Fuel | V-Based |
| Configuration 09 | 1 | 0 | $NH_3$ | V-Based |

## 5 Results and Discussion

### 5.1 Vehicle and Engine Simulation Results

Figure 4 shows the effect of both ϕ and EGR rate on modelled polluting emissions (in g/km), namely $NO_x$, $N_2O$ and $NH_3$ based on WLTC cycle; the level obtained in [37] with E5 fuel is also indicted in the figures. The EGR rate positively affects $NO_x$ emissions since it drastically reduces the combustion temperature. However, it can create a loss of stability that will have a negative effect on both unburnt $NH_3$ and $NO_x$ emissions. Moreover, the equivalence ratio also strongly affects pollutant emissions (Figure 5), where a clear trade-off is shown for unburnt ammonia and $NO_x$: a maximum of $NO_x$ emissions at an equivalence ratio of 0.8 and unburnt ammonia for a very rich mixture.

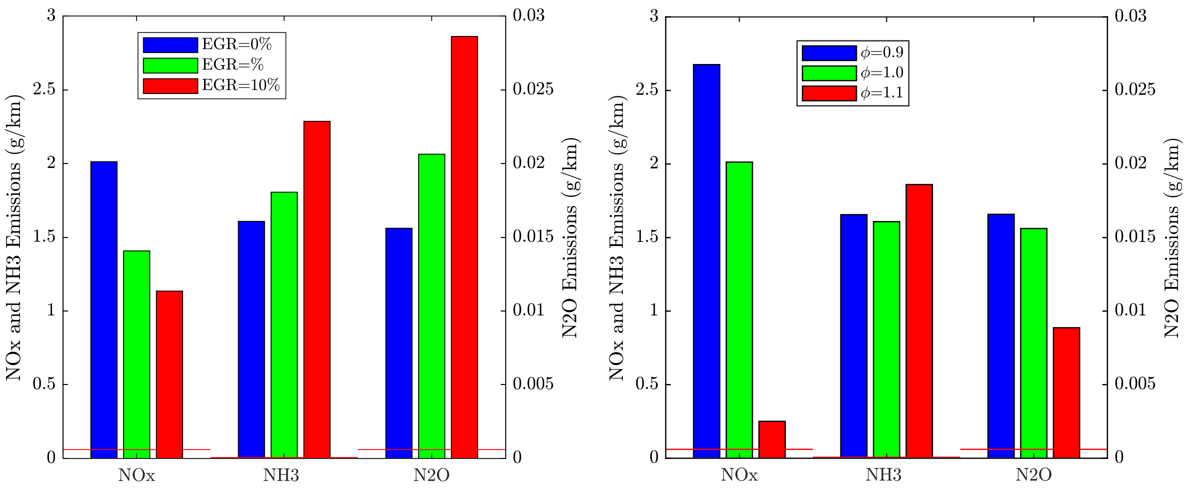



*Figure 4: a) Effect of EGR rate on pollutant emissions at stoichiometry. b) Effect of equivalence ratio on pollutant emissions without EGR rate.*

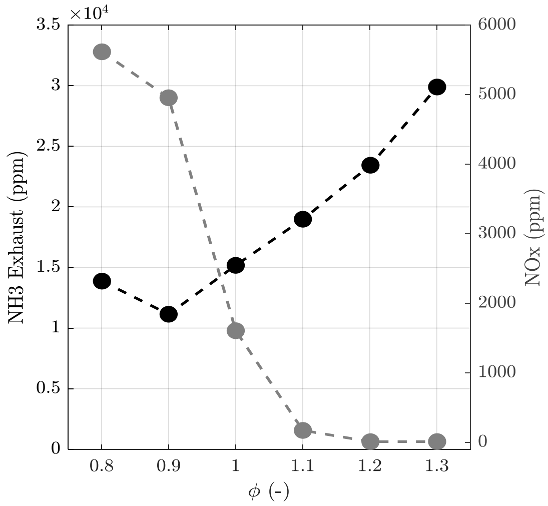



*Figure 5: Effect of equivalence ratio on NOx and NH3 exhaust emissions*

Pollutant emissions were modelled right after the SCR system as a function of the SCR technology and were compared to the level obtained with E5 fuel (red line), Figure 6a. Finally, even if an Ammonia Oxidation Catalyst (AOC) model is added along the exhaust line, the level of $NH_3$ emission remains above the regulation limit. The unit aims to convert the excess ammonia at the exhaust using a constant clean-up catalyst with an efficiency of 95%. Figure 6.b summarises how each pollutant behaves along the modelled post-treatment exhaust line for the reference case (i.e. without EGR) at the stoichiometry (ϕ=1) and with a V-based SCR system.

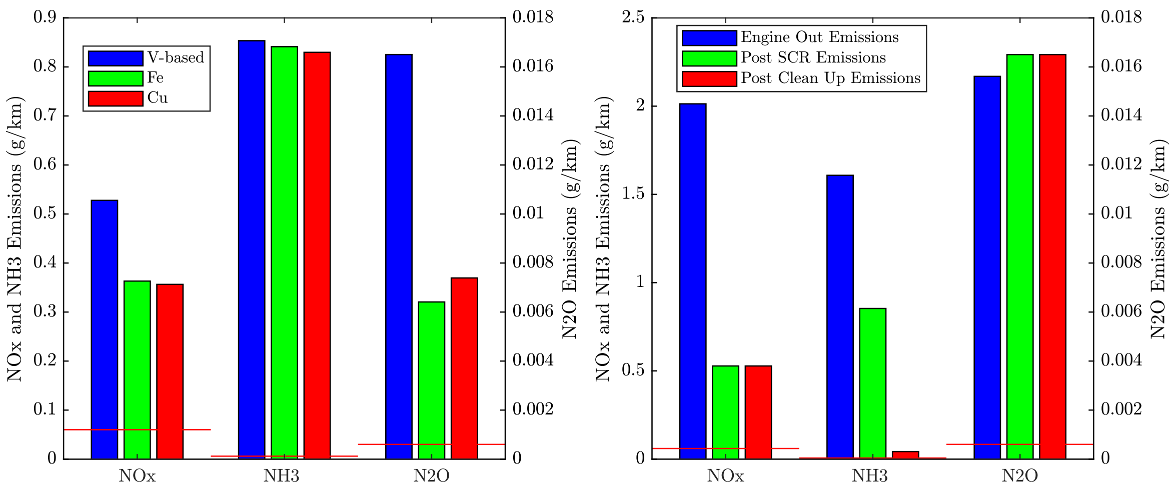



*Figure 6: a) Effect of SCR technology on the emissions at the output of the SCR. b) Emissions results, computed all along the exhaust line.*

Table 4 summarises the fuel consumption and exhaust emissions at the engine and after-treatment system, respectively. The after-treatment system has a higher effect on reducing $NH_3$ and $NO_X$ emissions, on average -97% and -75%, respectively. Whereas for $N_2O$ emissions, some strategies have an unfavourable effect, such as changes in the ER and fuel-based gearbox optimisation criteria, which result in higher $N_2O$ emissions. A Fe-based and Cu-based SCR have better performance in pollutant emissions reduction, -97% in $NH_3$, between -59% and -53% in $N_2O$, and -82% in $NO_X$.

*Table 4: Fuel consumption and air emissions from an ammonia-based ICE vehicle*

| Configurations | Fuel consumption (l/ 100 km) | Engine out emissions (kg/km) | | | Post clean up emissions (kg/km) | | |
|---|---|---|---|---|---|---|---|
| | | $NH_3$ | $N_2O$ | $NO_X$ | $NH_3$ | $N_2O$ | $NO_X$ |
| Conf 01 | 13.8431 | $1.61x10^{-3}$ | $1.56x10^{-5}$ | $2.01x10^{-3}$ | $4,27x10^{-5}$ | $1,65x10^{-5}$ | $5,28x10^{-4}$ |
| Conf 02 | 13.9801 | $1.66x10^{-3}$ | $1.66x10^{-5}$ | $2.67x10^{-3}$ | $3,11x10^{-5}$ | $1,80x10^{-5}$ | $7,10x10^{-4}$ |
| Conf 03 | 13.9988 | $1.86x10^{-3}$ | $8.87x10^{-6}$ | $2.49x10^{-4}$ | $9,36x10^{-5}$ | $1,31x10^{-5}$ | $6,57x10^{-5}$ |
| Conf 04 | 14.9389 | $1.81x10^{-3}$ | $2.06x10^{-5}$ | $1.40x10^{-3}$ | $6,64x10^{-5}$ | $1,94x10^{-5}$ | $3,69x10^{-4}$ |
| Conf 05 | 16.9256 | $2.29x10^{-3}$ | $2.86x10^{-5}$ | $1.13x10^{-3}$ | $9,74x10^{-5}$ | $2,41x10^{-5}$ | $2,98x10^{-4}$ |
| Conf 06 | 13.8431 | $1.61x10^{-3}$ | $1.56x10^{-5}$ | $2.01x10^{-3}$ | $4,21x10^{-5}$ | $6,41x10^{-6}$ | $3,63x10^{-4}$ |
| Conf 07 | 13.8431 | $1.61x10^{-3}$ | $1.56x10^{-5}$ | $2.01x10^{-3}$ | $4,15x10^{-5}$ | $7,39x10^{-6}$ | $3,56x10^{-4}$ |
| Conf 08 | 13.8361 | $1.88x10^{-3}$ | $2.23x10^{-5}$ | $2.42x10^{-3}$ | $4,71x10^{-5}$ | $1,70x10^{-5}$ | $7,87x10^{-4}$ |
| Conf 09 | 13.8431 | $1.61x10^{-3}$ | $1.56x10^{-5}$ | $2.01x10^{-3}$ | $4,27x10^{-5}$ | $1,65x10^{-5}$ | $5,28x10^{-4}$ |

It should be noted that the emissions profile for configurations 06 and 07 at engine exhaust (scenario without after-treatment system) is the same as the base case (configuration 01). Configurations 06 and 07 are models in which the SCR is based on Fe and Cu-exchanged zeolites instead of V-based catalysts.

### 5.2 Life Cycle Impact Assessment

Table 5 shows the impact characterisation of the ammonia-based passenger car, considering the exhaust emissions without and with the after-treatment system.

*Table 5: LCIA Results for ammonia-based ICE vehicle (Functional unit: 1 km travelled)*

| | Climate change **GWP100** (kg $CO_2$-eq) | Fossil depletion **FDP** (kg Oil-eq) | Freshwater eutrophication **FEP** (kg P-eq) | Ozone depletion **ODPinf** (kg CFC-11-eq) | Photochemical oxidant formation **POFP** (kg NMVOC-eq) | Terrestrial acidification **TAP100** (kg $SO_2$-eq) |
|---|---|---|---|---|---|---|
| | **Without after-treatment system** | | | | | |
| Conf01 | $9.80x10^{-2}$ | $3.07x10^{-2}$ | $3.89x10^{-5}$ | $8.89x10^{-9}$ | 2.47x10-3 | $5.70x10^{-3}$ |
| Conf02 | $9.84x10^{-2}$ | $3.07x10^{-2}$ | $3.89x10^{-5}$ | $8.90x10^{-9}$ | 3.13x10-3 | $6.19x10^{-3}$ |
| Conf03 | $9.61x10^{-2}$ | $3.07x10^{-2}$ | $3.89x10^{-5}$ | $8.90x10^{-9}$ | 7.10x10-4 | $5.33x10^{-3}$ |
| Conf04 | $1.00x10^{-1}$ | $3.08x10^{-2}$ | $3.91x10^{-5}$ | $8.93x10^{-9}$ | 1.87x10-3 | $5.86x10^{-3}$ |
| Conf05 | $1.03x10^{-1}$ | $3.09x10^{-2}$ | $3.93x10^{-5}$ | $8.99x10^{-9}$ | 1.59x10-3 | $6.93x10^{-3}$ |
| Conf06 | $9.80x10^{-2}$ | $3.07x10^{-2}$ | $3.89x10^{-5}$ | $8.89x10^{-9}$ | 2.47x10-3 | $5.70x10^{-3}$ |
| Conf07 | $9.80x10^{-2}$ | $3.07x10^{-2}$ | $3.89x10^{-5}$ | $8.89x10^{-9}$ | 2.47x10-3 | $5.70x10^{-3}$ |
| Conf08 | $1.00x10^{-1}$ | $3.07x10^{-2}$ | $3.89x10^{-5}$ | $8.89x10^{-9}$ | 2.88x10-3 | $6.59x10^{-3}$ |
| Conf09 | $9.80x10^{-2}$ | $3.07x10^{-2}$ | $3.89x10^{-5}$ | $8.89x10^{-9}$ | 2.47x10-3 | $5.70x10^{-3}$ |
| | **With after-treatment system** | | | | | |
| Conf01 | $9,83x10^{-2}$ | $3,07x10^{-2}$ | $3,89x10^{-5}$ | $8,89x10^{-9}$ | $9,88x10^{-4}$ | $1,03x10^{-3}$ |
| Conf02 | $9,88x10^{-2}$ | $3,07x10^{-2}$ | $3,89x10^{-5}$ | $8,90x10^{-9}$ | $1,17x10^{-3}$ | $1,11x10^{-3}$ |
| Conf03 | $9,73x10^{-2}$ | $3,07x10^{-2}$ | $3,89x10^{-5}$ | $8,90x10^{-9}$ | $5,27x10^{-4}$ | $9,02x10^{-4}$ |
| Conf04 | $9,96x10^{-2}$ | $3,08x10^{-2}$ | $3,91x10^{-5}$ | $8,93x10^{-9}$ | $8,31x10^{-4}$ | $1,02x10^{-3}$ |
| Conf05 | $1,02x10^{-1}$ | $3,09x10^{-2}$ | $3,93x10^{-5}$ | $8,99x10^{-9}$ | $7,63x10^{-4}$ | $1,10x10^{-3}$ |

| | Climate change **GWP100** (kg $CO_2$-eq) | Fossil depletion **FDP** (kg Oil-eq) | Freshwater eutrophication **FEP** (kg P-eq) | Ozone depletion **ODPinf** (kg CFC-11-eq) | Photochemical oxidant formation **POFP** (kg NMVOC-eq) | Terrestrial acidification **TAP100** (kg $SO_2$-eq) |
|---|---|---|---|---|---|---|
| Conf06 | 9,53x10$^{-2}$ | 3,07x10$^{-2}$ | 3,89x10$^{-5}$ | 8,89x10$^{-9}$ | 8,24x10$^{-4}$ | 9,39x10$^{-4}$ |
| Conf07 | 9,56x10$^{-2}$ | 3,07x10$^{-2}$ | 3,89x10$^{-5}$ | 8,89x10$^{-9}$ | 8,17x10$^{-4}$ | 9,34x10$^{-4}$ |
| Conf08 | 9,84x10$^{-2}$ | 3,07x10$^{-2}$ | 3,89x10$^{-5}$ | 8,89x10$^{-9}$ | 1,25x10$^{-3}$ | 1,19x10$^{-3}$ |
| Conf09 | 9,83x10$^{-2}$ | 3,07x10$^{-2}$ | 3,89x10$^{-5}$ | 8,89x10$^{-9}$ | 9,88x10$^{-4}$ | 1,03x10$^{-3}$ |

The after-treatment system significantly diminishes $NH_3$ and $NO_X$ emissions in all configurations; hence, the indicators associated with these emissions, POFP and TAP100, show a comparable reduction, about -56% and -82%, respectively (Figure 7). The variance without and with the after-treatment system is negligible for the other indicators.

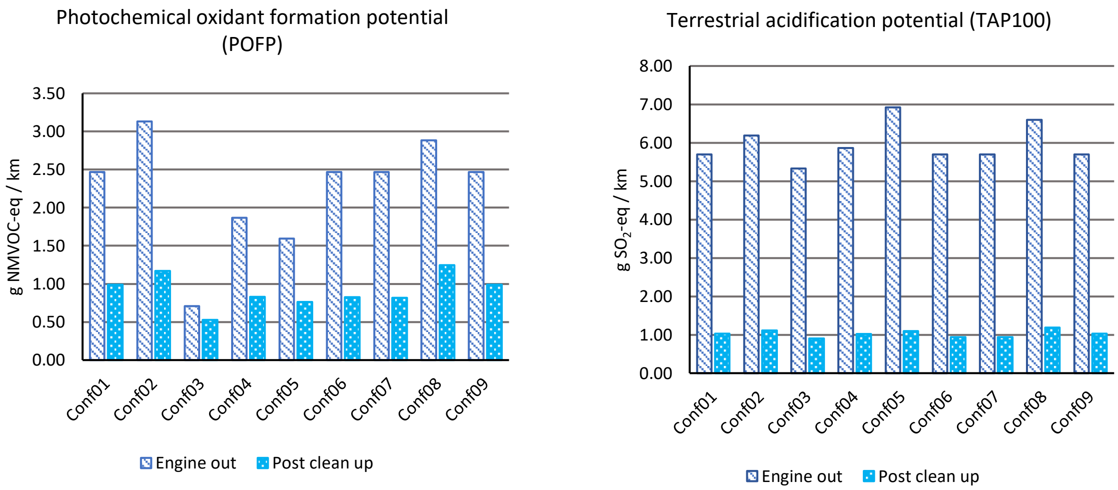



*Figure 7: Comparison of impact category indicators Photochemical oxidant formation potential (POFP) and Terrestrial acidification potential (TAP100) without and with an after-treatment system*

The variability in the LCA results among configurations is associated with vehicle operating conditions, Figures 8 and 9. An ammonia-based passenger car's carbon footprint (GWP) fluctuates depending on $N_2O$ emissions, ranging from 0.095 to 0.102 kg $CO_2$-eq per km travelled. Fossil depletion, freshwater eutrophication, and ozone depletion potential do not oscillate considerably. However, some correspondence with ammonia consumption is observed; due to the use of fossil fuels in the distribution of ammonia and certain emissions associated with the construction of the transmission network for the electricity needed to produce ammonia. The photochemical oxidant formation potential changes depending upon $NO_X$ emissions (Figure 9e), likewise for terrestrial acidification potential (Figure 9f). However, the emissions of $NH_3$ during operation also contribute to acidification.

Regarding climate change, Configurations 06 and 07 (using Fe and Cu-exchanged zeolites for SCR) correspond to the lowest burden to the environment; in contrast, Configuration 05 corresponds to a larger carbon footprint. Configuration 05 also entails the highest fuel consumption; therefore, the impact categories of fossil depletion, freshwater eutrophication, and ozone depletion potential are slightly higher than the other configurations, where the values for these indicators remain constant.

Configuration 03, with an equivalence ratio of 1.1, denoted the lowest $NO_X$ emissions, although it has better performance regarding photochemical oxidant formation and terrestrial acidification. This result agrees with a previous study by Razon and Valera-Medina on an ammonia-fuelled gas turbine for power generation [15].

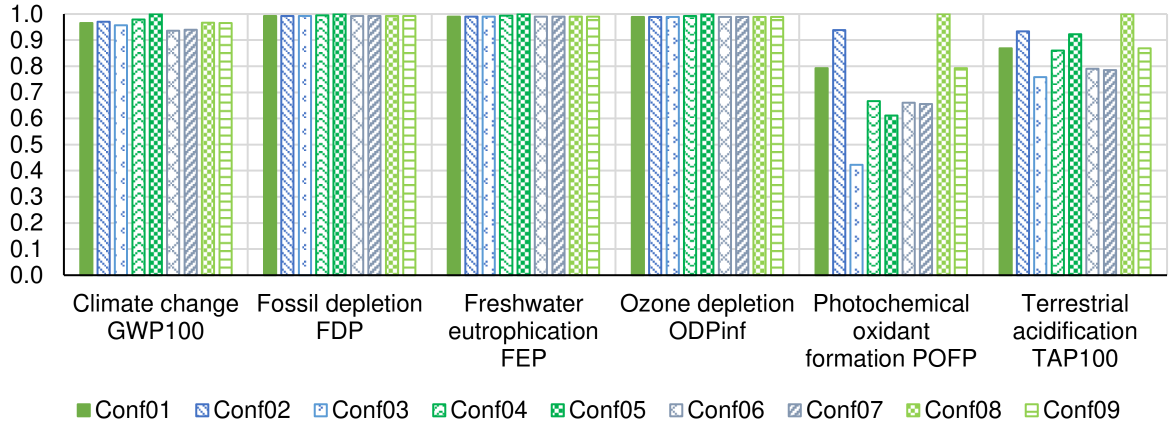
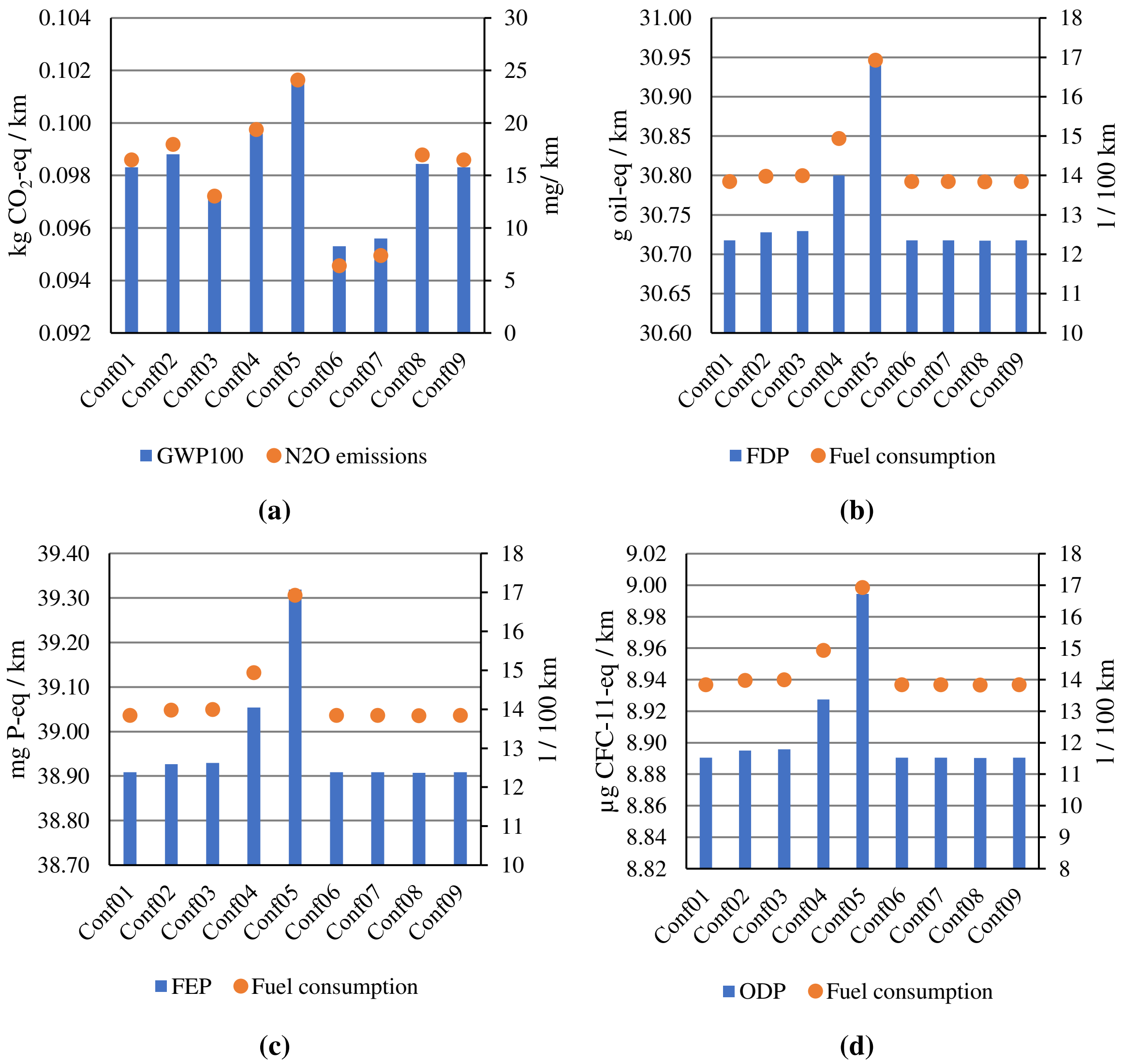
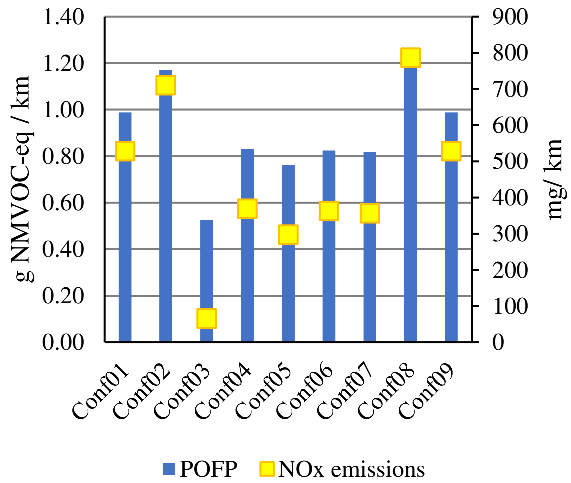
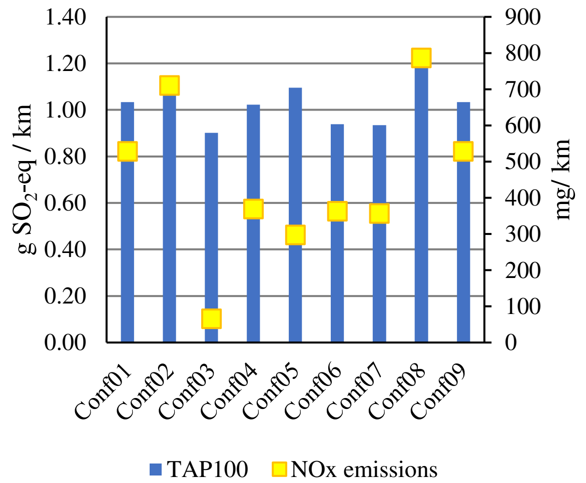



*Figure 8: Impact category indicators variation between configurations (post-clean-up)*





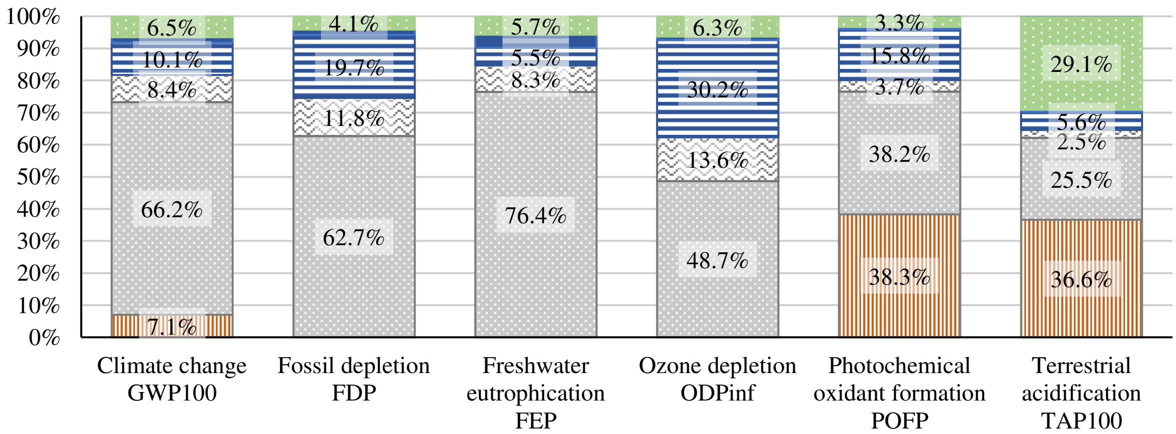

**(e)**



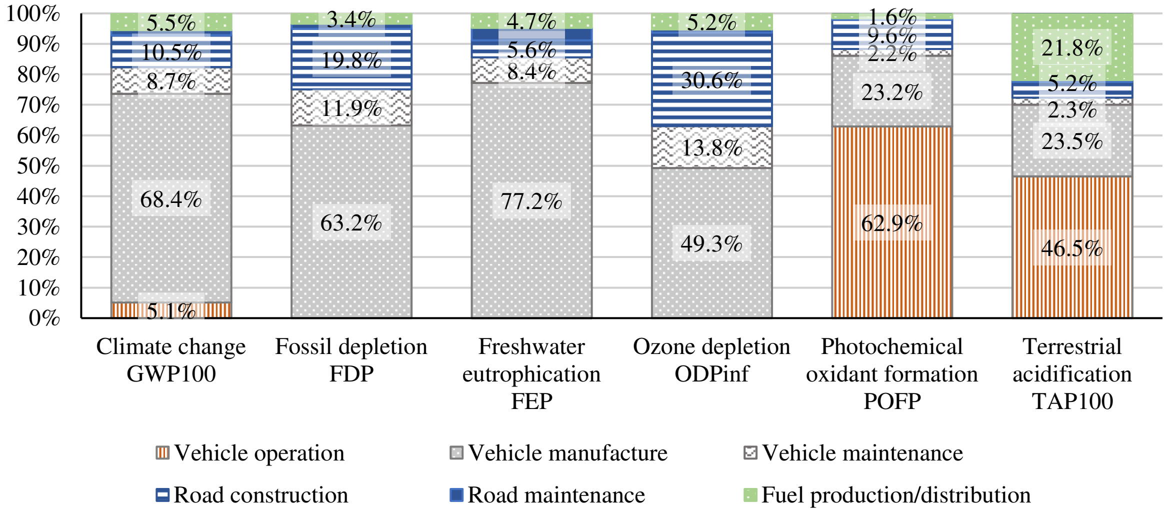

**(f)**

*Figure 9: Impact category indicators results for an ammonia-based passenger car in function with exhaust emissions (post-clean-up). (a) Global warming potential (GWP100), (b) Fossil depletion potential (FDP), (c) Freshwater eutrophication potential (FEP), (d) Ozone depletion potential (ODP), (e) Photochemical oxidant formation potential (POFP), (f) Terrestrial acidification potential (TAP100).*

The contribution analysis for the impact categories included in this work (Figure 10) shows that the operation phase is negligible for the impact categories FDP, FEP, and ODP, whilst for Carbon Footprint, GWP100, the contribution is minimal (7.1% or lower across all configurations). The operation phase is more relevant for photochemical oxidant formation and terrestrial acidification potential. For the POFP, the $NO_X$ emissions' effect during the vehicle's operation can be as high as 63% (Config 8). Likewise, the operation phase for terrestrial acidification, due to the emissions of $NO_X$ and $NH_3$, represents a considerable share.




**(a)**




**(b)**

*Figure 10: Contribution analysis for the impact category indicators results of 1 km travelled (post-clean-up). (a) Configuration 5, (b) Configuration 8*

A comparison with gasoline and diesel-fuelled vehicles is performed to evaluate the environmental sustainability of ammonia as an alternative fuel for passenger transportation (Figures 11 and 12). There is a noticeable reduction in global warming, fossil depletion, and ozone depletion potential (such as -71%, -70%, and -81% in comparison with a gasoline engine vehicle for GWP100, FDP, and ODP, respectively). The impact category of freshwater eutrophication is mainly related to the phosphates emissions during waste treatment processes associated with obtaining materials for vehicle manufacturing; therefore, there is no significant difference in this impact category.

Compared with gasoline and diesel ICE cars, using ammonia represents a higher burden for terrestrial acidification potential across all configurations. Regarding the photochemical oxidant formation potential, only for Configuration 03 (ER = 1) is there a reduction (-26%); however, considering other operation modes and control pollution strategies, the associated impact of the ammonia-fuelled engine is higher than conventional fossil-fuelled ICE (from 7% for Config05 to 76% for Config08).

Ammonia-based ICE vehicles represent a trade-off between climate change potential and photochemical oxidant formation, and terrestrial acidification potential; this could be relevant for locations with smog problems. Consequently, as has been mentioned in the literature [3,38] a combination of emissions abatement technologies and policies is needed to diminish the effect of $NO_X$ and $NH_3$ emissions on the environment.

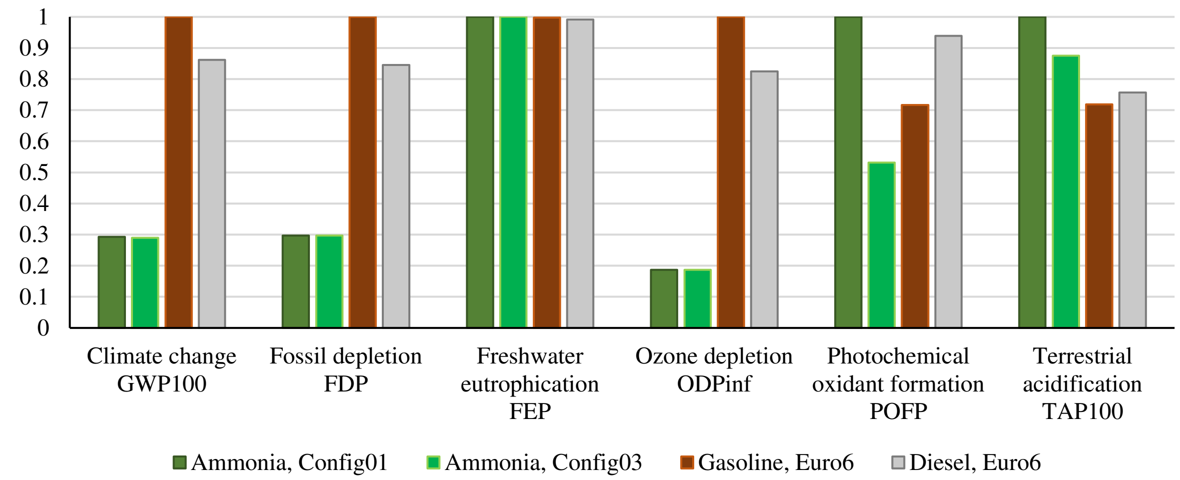



*Figure 11: Life cycle impact comparison for a passenger vehicle using ammonia, gasoline, and diesel*

Figure 12 shows the contribution analysis for the impact category of global warming potential by comparing the three types of vehicles. There is a reduction in GHG emissions not only during the operation phase (-97%) but also in fuel production and distribution (-85% in comparison with gasoline and -76% with diesel). The other processes (i.e., vehicle manufacturing and maintenance, road construction and maintenance) are the same for the three vehicles. The reduction in GHG emissions during the operation phase results in a hotspot shift to manufacturing; the same has been observed in exploring strategies to decarbonise the built environment and other energy carriers in the transportation sector (hydrogen and electric vehicles) [39,40]. Consequently, the research focus for further decarbonisation would be on manufacturing processes and embodied carbon in materials.

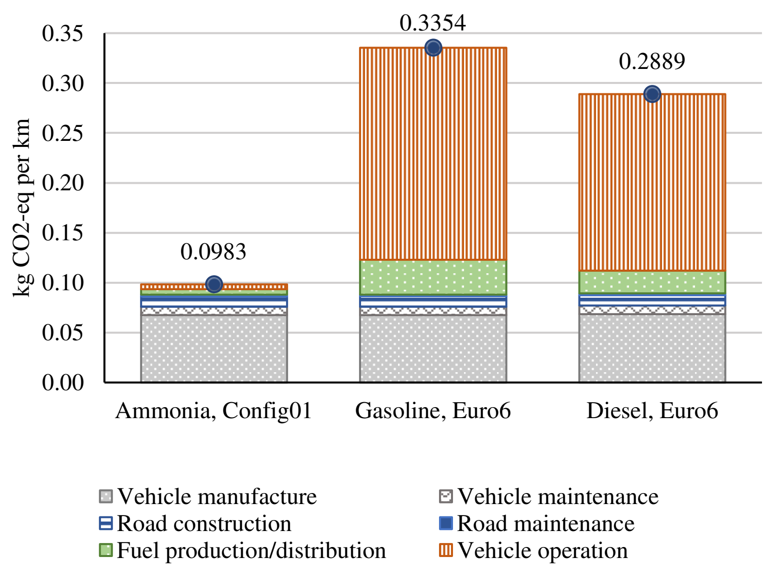



*Figure 12: Contribution analysis and comparison of the Global Warming Potential of a 1 km travelled by passenger car using ammonia, gasoline, and diesel*

There are few studies in the literature assessing the environmental sustainability of ammonia [10,14] and ammonia blends with fossil fuels [8] in ICEV for passenger transportation. Figure 13 compares the carbon footprint of the results found in the literature and those shown in this study. For this study, a sensitivity analysis considering various types of ammonia (different feedstock and energy sources for ammonia production and production locations) is incorporated based on the LCI developed in a previous research paper [17]. Regarding lifecycle GHG emissions, the use of green ammonia (electrolysis for $H_2$ production using renewable energy), blue (steam methane reforming for $H_2$ production with CCS), or pink (electrolysis for $H_2$ production using nuclear) represents a lesser burden than gasoline and diesel vehicles for passenger transportation. Even though the use of grey ammonia ($H_2$ production from methane through the steam methane reforming process) shows a comparable impact to diesel and gasoline fuelled cars. As supported by the research on the environmental friendliness of ammonia as an energy carrier in other systems [12,13,20,21], ammonia must be produced from renewable resources to provide environmental benefits compared to traditional fossil-based energy carriers.

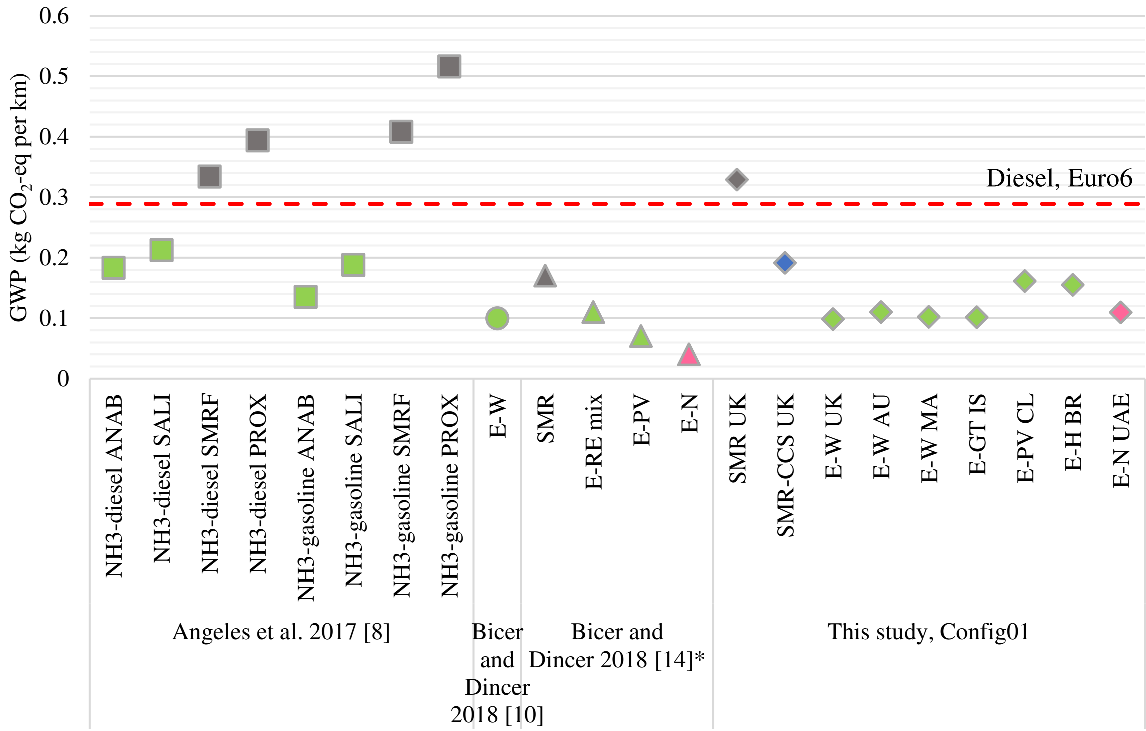



*Figure 13. Comparison of the Global Warming Potential of 1 km travelled on ammonia and ammonia blends with fossil fuels ICE vehicles. Notes: *GWP estimation over 500 years period. ANAB: cyanobacterial process, SALI: wood-based process, SMRF: Steam reforming, PROX: partial oxidation, RE: renewable energy, SMR: steam methane reforming, CCS: carbon capture and storage, E: electrolysis, W: wind energy, GT: geothermal energy, PV: photovoltaic, H: hydropower, N: nuclear, UK: The United Kingdom, AU: Australia, MA: Morocco, IS: Iceland, CL: Chile, BR: Brazil, UAE: United Arab Emirates.*

It is noticeable that using blends (between 40-60% of ammonia with diesel [8]) with fossil fuel in ICEV, as long as the ammonia is produced from renewable energy, results in comparable values with the use of ammonia alone in terms of carbon footprint. Regarding other impact categories, the results of this study agree with those from the literature [10,12,14], where there is a reduction in ozone layer depletion and an increase in acidification related to a conventional fossil-based ICEV.

## 5.3 Limitations and recommendations for further research

Although modelling the vehicle operation considering different configurations sheds light on which strategies are the most suitable to reduce emissions, it is necessary to validate these results with actual road data. Consequently, an update of the life cycle impact assessment of the ammonia-based vehicle is in order when this data is available.

As mentioned in previous studies of the literature, as well as the results of this study support the use of green ammonia as an alternative for passenger transport, with less environmental burden in comparison with conventional fuels. However, further research in these early stages is needed for a successful commercial deployment to improve the product system's overall energy and exergy efficiencies. Therefore, developing a life cycle energy and exergy analysis coupled with environmental LCA and life cycle costing of the ammonia fuelled ICEV and comparing it with other novel fuels/technologies will help to identify the sustainability issues and trade-offs.

# 6 Conclusions

The environmental sustainability of ammonia as an alternative fuel for private passenger transportation was evaluated from a life cycle perspective. An emissions profile of the SI engine fuelled with ammonia was developed at the post-engine and post-clean-up system. The after-treatment system noticeable reduces pollutant exhaust emissions; however, these remain above the regulation limits. Nine configurations for the engine were modelled to optimise fuel consumption and minimise exhaust emissions; catalysts based on Fe and Cu-exchanged zeolites perform better in emissions reduction. Consequently, their incorporation in the after-treatment system positively affects the lifecycle environmental profile of ammonia-based passenger transportation.

The operation of an ammonia-based vehicle has a small contribution to its carbon footprint; therefore, other processes, such as vehicle manufacturing and maintenance, and road construction, become more relevant. As the operation becomes more efficient in terms of GHG emissions reduction, to further diminish the transport sector's contribution to global warming, it is necessary to look out for strategies to implement in the upstream processes to reduce its carbon footprint as well.

Photochemical oxidant formation potential (POFP) and terrestrial acidification potential (TAP100) are more sensitive to vehicle operation than the other four indicators studied. $NO_X$ and $NH_3$ direct emissions during vehicle operation are the higher contributors to these impacts. Further research on optimisation engine strategies and pollution control is needed to cap the burden associated with $NO_X$ and $NH_3$ emissions from ammonia combustion.

Comparing an ammonia-based passenger vehicle versus a conventional ICE vehicle using fossil fuels, gasoline, and diesel, the environmental profile of the former seems more favourable. Therefore, ammonia-based transportation could have an essential role in the range of options to contribute to the decarbonisation of the transport sector.

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