Potential Pollutant Emission Effects of Connected and Automated Vehicles in a Mixed Traffic Flow Context for Different Road Types

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ABSTRACT The environmental impact of connected and autonomous vehicles (CAVs) is still uncertain. Little is known about how CAVs operational behavior influences the environmental performance of network traffic, including conventional vehicles (CVs). In this paper, a microscopic traffic and emission modeling platform was applied to simulate CAVs operation in Motorway, Rural, and Urban road sections of a medium-sized European city, assuming different configurations of the car-following model parameters associated with a pre-determined or cooperative adaptative behavior of the CAVs. The main contribution is to evaluate the impact of the CAVs operation on the distribution of accelerations, Vehicle Specific Power (VSP) modal distribution, carbon dioxide (CO_2) and nitrogen oxides (NOx) emissions for different road types and Market Penetration Rates (MPR). Results suggest CAVs operational behavior can affect CVs environmental performance either positively or negatively, depending on the driving settings and road type. It was found network-wide CO_2 varies between savings of 18% and an increase of 4%, depending on the road type and MPR. CAVs adjusted driving settings allowed minimization of system NOx up to 13-23% for MPR ranging between 10 and 90%. These findings may support policymakers and traffic planners in developing strategies to better accommodate CAVs in a sustainable way.

INDEX TERMS Car-following adjustment parameters, connected and automated vehicles, driving behavior, microsimulation, pollutant emissions.

I. INTRODUCTION

URBAN population growth and the challenges related to climate change are important reasons to move towards a more sustainable transport system. In Europe, road transport is responsible for more than 70% of total carbon dioxide (CO_2) emissions, with passenger cars being the major contributor [1]. Despite recent technological and emission standard regulations, last data showed emission reductions from road transport have been lower

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than originally anticipated, partly because of the growth in transport demand [2]. For certain pollutants, such as nitrogen oxides (NOx), there has been an increase associated with diesel vehicles [2]. Furthermore, according to the International Energy Agency, consumers are buying ever larger and less fuel-efficient cars such as Sport Utility Vehicles - SUVs [3]. The European Environment Agency (EEA) reported that average CO_2 emissions from new passenger cars registered in the European Union (EU) increased again in 2019 [4].

Moreover, an increasing preponderance of plug-in hybrid cars in electric car sales and the corresponding decrease in

the share of 100% electric cars are being observed. Even in optimal test conditions, PHEV emissions are 28-89% higher than advertised [5]. In 2019, hybrid electric vehicles (HEV) represented more than 55% of alternatively-powered vehicles sold in the EU and 6% of new-car registrations [6]. Overall, vehicle tailpipe emissions above standards are associated with almost 40,000 deaths globally in 2015, including approximately 10% of all ozone-related premature deaths in the European Union [7]. Thus, road transport continues to play an important role in climate change and human health impacts.

Significant change lies ahead for the transport sector due to the deployment of cooperative intelligent transport systems (C-ITS) and progressive implementation of vehicles with an increasing degree of autonomy. These technologies are expected to improve the transport system's performance and reduce human errors [8], [9]. Eventually, automated operational and strategic systems can be implemented to reduce negative environmental impacts by impacting the surrounding conventional vehicles (CVs). Since connected and automated vehicles (CAVs) will inevitably share the roads with CVs for a long period, it is timely to study the network-wide potential impacts of different market penetration rates (MPR) of CAVs [10]. By operating under optimized driving behavior settings for different road types, pollutant emissions as CO_2, associated with climate change impacts, and NOx emissions associated with air quality and health impacts may be minimized. Therefore, the goal of the present study is to examine CAVs operational behavior influence in the system-wide environmental performance. The innovative nature of the study relies on the testing of several possibilities that could be used in future logic controls for CAVs, assuming i) an expected configuration available in previous studies; and ii) an optimized driving behavior to minimize NOx emissions in an urban context. Based on a microsimulation platform, the operational impact of CAVs is examined through a detailed analysis of the kinematics (e.g., acceleration) and Vehicle Specific Power (VSP) patterns, and pollutant emissions of the different categories of vehicles circulating in the network.

The remainder of this paper is organized as follows. Section II introduces previous research in what respects the simulation of CAVs driving behavior on mixed traffic road systems followed by the impact of CAVs operation on network efficiency and environmental performance. This section finishes by outlining the main research gaps. Section III is devoted to describing the methodology used to address the answers to the proposed research questions. In Section IV, results obtained using the simulation-based framework applied to three different road types are presented and discussed for different MPR of CAVs. A detailed analysis of the urban road case is given, and some consequences of the methodological approach are addressed at the end of Section IV. The last section ends with concluding remarks, paper contributions, and future research directions (Section V).

II. LITERATURE REVIEW
A. ASSESSING CAVS DRIVING LOGIC IN MIXED TRAFFIC FLOWS
The increasing interest in capturing the effect of the different driving logics between CVs and CAVs has heightened the need for detailed studies on vehicles interaction [11]. Most studies rely on simulation-based frameworks due to the lack of CAVs real-world data ([12]–[13]). Nevertheless, there have been proposed some empirical studies based on pilot assessments with very limited empirical data and relying on platoon compositions. For instance, in [14], controllers were developed to achieve significant reductions in inter-vehicular gaps. These were tested in a platoon of four vehicles on a highway and results showed improvements in response time, highway capacity, and traffic flow stability. In [15], empirical experiments with a platoon of low-level automated vehicles were conducted, mainly focusing on the interaction of the platoon in traffic. It was found that the benefits of the platoon strongly depend on the traffic conditions and that for low-level automated vehicles large platoons turn to cause instabilities in the car-following behavior. Driving interactions between automated vehicles and CVs were explored in [16] through an experimental study focusing on platoon car-following behavior. Simulation results for a MPR of 50% showed CVs could drive closer to automated vehicles. However, to develop a robust model of the interactions more empirical data are needed. In [17], field experiments using a single autonomous vehicle were conducted to assess its introduction effects to dampen traffic waves on a circular ring with several CVs. In the CoExist Project [18], CAVs were modeled based on data from a pilot case which were used to calibrate car-following models under the VISSIM [13] traffic simulator environment.

B. IMPACTS OF CAVS ON NETWORK EFFICIENCY
It has been shown that CAVs can significantly improve safety [19]–[21], traffic efficiency [22]–[24], traffic flow stability [11], and air quality [17], [25]. A recent comprehensive study has shown that it is important to take an adaptive approach to autonomous vehicles concerning the environmental impact. Its deployment can bring emission reductions or be a disaster, which will deeply depend on public policies [26]. At the operational level, CAV technologies are expected to improve fuel economy [27] and reduce emissions per unit of distance thanks to fewer stop-and-go movements [28] and due to more gradual acceleration and deceleration patterns [29]. Due to its lower reaction time compared to CVs, an increase in road capacity is expected due to short following distances [30], [31]. It has been shown that for freeway corridors with dedicated lanes for CAVs, benefits can be obtained in terms of the overall corridor performance metrics with increasing penetration rates up to 50%. However, it deteriorates considerably after these values [32]. In fact, the effects on vehicle miles traveled from various CAV technologies are not clear. Some studies highlighted induced demand for personal automobile travel [33],

due to empty trips, migration effects from other modes of transport, and potential low costs [34], [35]. Nevertheless, incorporating shared driverless cars can significantly reduce the total travel demand [33], [36] and annual vehicle distances traveled [37], [38]. With the introduction of CAVs, an improvement in traffic can be expected through more efficient driving, congestion relief, better accident prevention with a reduction estimated to be around 90%, as well as a reduction in fuel consumption, energy, and pollution up to 40% [20], [21]. Previous research has shown that a reduction of 12-17% in fuel use can be achieved when a CAV is trailing a lead vehicle with the specific objective of minimizing accelerations and decelerations [39]. A study conducted in the United States (US) showed reductions between 30 to 45% due to transitioning from CV to CAV fleets [40]. It was recently demonstrated that CAVs introduction could lead to significant progress towards EU emission targets, even for lower MPR and a decrease up to 19% on CO_2 emissions can be achieved in a 100% CAVs scenario [41]. Nevertheless, the projected environmental benefits of automation are not deeply understood yet, and various studies have highlighted some concerns, which reinforces the need for thoroughly exploring the influence of CAVs gradual introduction in the road infrastructures. For instance, automated vehicles could reduce traffic speeds and force the engines to work in less efficient spaces, which yield an increase in emissions [42] and may deteriorate the network performance [43]. Recently, research on the impacts of automated and cooperative systems in mixed traffic showed that CAVs could lead to higher fuel consumption and emission levels because of sharper accelerations of CAVs compared to CVs [43]. It was also shown automated vehicles generate the highest CO_2 emissions values per kilometer and CAVs generate more absolute emissions during peak-hours due to increased network capacity.

C. SIMULATION OF CAVS OPERATION

Considerable research efforts have been devoted to understanding how driving behavior parameters of CAVs affect infrastructure capacity, energy consumption, and emissions. Traffic-modeling parameters are rarely tested against real data for two reasons: first, data is not widely available, since car industry manufacturers have very restrictive data sharing policies; and second, technology is still under development [44], [45]. Some specific models have been proposed to reflect CAVs driving behavior. For instance, in [46], a uniform local platoon for stability analysis of CAV mixed-flow was proposed. It was simulated on a highway segment. The VT Micro and the VSP models were used to estimate emissions. Considering different MPR of CAVs, results show reductions ranging between 15 and 46% can be obtained for fuel consumption and emissions (carbon monoxide (CO), hydrocarbons (HC), and NOx), following an increasing trend with MPR. In [47], a comparison of CVs simulated using the Wiedemann99 model, with CAVs simulated using the MIXIC algorithm [48] was conducted

in the microsimulation tool VISSIM for a highway section. The emissions were estimated by MOVES. Reductions in the NOx emissions were around 3% and a slight increase was found for CO_2. In [49], CAVs were simulated under different MPRs and traffic demands in an urban center using the E2ECAV algorithm. Network-wide emissions reductions were higher as the MPR and travel demand increases, reaching savings around 39% in Greenhouse Gases (GHG) emissions and 10% in NOx. Nevertheless, a large body of literature has focused on adapting the Wiedemann car-following model from VISSIM. The CoExist Project showed this latter approach could be an alternative, which can be easily implemented within the traffic simulator VISSIM to perform scenario-based evaluations to assess variations in parameters under typical traffic situations [18]. In fact, this approach has been followed by various researchers ([44], [50], [51]). Hence, due to the absence of real-based data on the car-following algorithms used in the CAV industry, a frequently used approach to explore and anticipate CAVs impacts is to modify the current Car-Following Parameters (CFP) and adapt lane change models in the traffic simulation and modeling platforms to simulate the impact of CAVs operation on the network [52]. In some studies, it is assumed that CAVs can incorporate car-following adaptive algorithms to achieve secondary objectives such as minimizing emissions [51], [53], improve safety and mobility [23]. Other works attempt to anticipate the behavior of CAVs [24], [53]–[55] under different connectivity and automation levels [56], and connectivity with the leading vehicle and driving logics [18], [45]. For simulating CAVs driving movements, many studies have been conducted based on adjusting CFP from the PTV VISSIM traffic simulation model [13], particularly under the Wiedemann 99 car-following model. This model is composed of nine parameters related to the standstill distance (CC0), headway time (CC1), following variation (CC2), the threshold for entering following (CC3), following thresholds (CC4/CC5), speed dependency of oscillation (CC6), oscillation acceleration (CC7), standstill acceleration (CC8) and acceleration at 80 km.h^{-1} (CC9) ([13], [61]). A great deal of emphasis has been placed on taking advantage of microscopic simulation tools for emulating the CAVs behavior as well as simulating their interactions within the road environment [44]. In particular, numerous studies have proposed to use the Wiedemann 99 car-following model and a suitable range of values for the above parameters to model CAVs in different types of roads and traffic conditions ([18], [23], [24], [45], [50], [51], [54], [55]). Considering the deterministic behavior of CAVs and to reflect much smaller fluctuation in vehicle longitudinal behavior, CC2 and CC6 parameters can be reduced to zero, as suggested by [18], [23], [45], [50], and [51]. Moreover, both CC4 and CC5 controlling speed differences during car-following can also be set to 0 m.s^{-1} when simulating CAVs ([23], [45]). Several Wiedemann 99 CFP influence density and road capacity. The CC0 is the average desired distance between two consecutive stopped vehicles affecting links

(i.e., road sections) and its default value is 1.50 m. Higher values (up to 4 m) are associated with the most cautions driving behavior [45], while lower values (0.25-0.5 m, depending on the road type) are typically found on most aggressive behavior ([18], [23], [24], [50], [51], [54]). CC1 controls the speed-dependent part of the desired safety distance. In links with high traffic flows, CC1 is the most important parameter affecting road capacity [61]. While the CC1 default value for CVs is 0.90 s, values assigned to CAVS in previous studies ranged between 0.4 s [24], [45] and 2 s [23]. Regarding CC3, this CFP determines the number of seconds before reaching the safety distance and controls the beginning of the deceleration process. Typically, CAVs were assigned to CC3 values ranging between -16.00 for cautious and -4.00 for a more assertive driving behavior ([50], [51]). The adopted CC7 values for simulating CAVs varied from 0.05 to 0.45 $(m.s^{-2})$, being the latter associated with more aggressive behavior [23]. The reference value of CC8 is 3.5 $m.s^{-2}$, but relevant studies assumed different levels of assertiveness ranging from -11% [23] up to $+20\%$ [55]. Concerning the CC9 (default value is 1.5 $m.s^{-2}$), the suggested values for CAVs driving behavior range from 1.1 $m.s^{-2}$ [23] up to 1.9 $m.s^{-2}$ [55].

Previous studies ([50], [51]) also devoted some attention to simulating CAVs in a mixed road environment by conducting a sensitivity analysis of the CFPs and analyzing the impacts on pollutant emissions. The findings from these studies indicated that the tunning of the parameters CC0, CC1, CC3, and CC8 were considered the most relevant in influencing the emissions emitted by vehicles.

D. RESEARCH GAPS

In summary, most of the existing literature focuses on assessing the impacts of CAVs deployment in terms of capacity, congestion, safety, fuel consumption, and CO_2 emissions [18], [35], [43], [44], [50]. However, few studies have focused on air quality impacts, mainly concerning NOx emissions [17], [18], [49]. Results found in the literature show that some benefits can be obtained for specific conditions. However, an integrated approach encompassing both climate change and health impacts in a coexistence environment of CAVs and CVs is not fully exploited. The purpose of this study is to pave the way for analyzing the possible impacts of CAVs introduction in current road infrastructures concerning both CO_2 and NOx emissions and evaluate these for different road types. In the first phase, literature reference values for CAVs driving behavior are adopted, and the associated environmental impacts are evaluated for different road types. The selected roads to explore the impacts of CAVs gradual implementation involved urban, national, and motorway segments, which yield differences regarding singularities, speed limits, and traffic volumes. In the second phase, the study focuses solely on the urban section and evaluates the optimal setting of CAVs CFPs that allow minimizing the system-wide NOx emissions. This is of great importance in terms of local air quality since the urban section involves various traffic singularities (e.g., signalized intersections and roundabouts) and higher air pollution exposure of residents and young students due to the proximity of schools to the major road. In this context, the evaluation of the best scenario seeking to minimize local emissions in the vicinity of the urban road is worthy of investigation to improve local air quality when CAVs will share the roads with CVs. For that purpose, the simulation of CAVs driving behavior was done by iteratively adjusting the Wiedemann 99 modified CFPs to find the optimal setting so that the network-wide NOx emissions, a local pollutant with demonstrated impacts on human health, are minimized.

This research is based on three fundamental questions not addressed yet in an integrated way in previous studies:

1) What is the variation of CO_2 and NOx emissions resulting from CAVs operation in different road typologies?
2) How do network-wide emissions vary for different MPR of CAVs?
3) What is the potential impact of CAVs on the environmental performance of CVs on different road types?

The answers to these questions are expected to yield insights on the environmental impacts of CAVs and CVs sharing the road infrastructure. This work can be relevant for planners and policymakers to understand the direction and magnitude of the potential consequences of CAVs, being important to support the development of strategies to better accommodate such new technologies.

III. METHODOLOGY

In this section, the methodology used in this work and details on the case study are presented. Fig. 1 shows the conceptual illustration of the followed methodology, and some assumptions are reported in Table 1.

Since real-world data related to CAVs are quite scarce, microsimulation appears as a relevant tool to investigate the potential impacts of their driving behavior [18], [35], [44], [50]. The present work relies on a microsimulation traffic platform to explore the impacts of CAVs circulating and sharing the roads with CVs. The developed model combines emission estimation with traffic microsimulation in a single platform to assess the impacts of CAVs gradual implementation on different road types. The methodology followed here (see Fig. 1) involves various steps. In the first step, field data on network design, fleet composition, traffic lights, and vehicles routes along three types of roads (urban, arterial, and motorway) have been gathered to reflect the network specificities and the baseline scenario. Then, under the VISSIM traffic simulator [13], CAVs and CVs need to be simulated in the traffic network. CVs are simulated based on default parameters, and fleet composition is adapted to represent local conditions in terms of traffic volumes, vehicle speed, and acceleration,
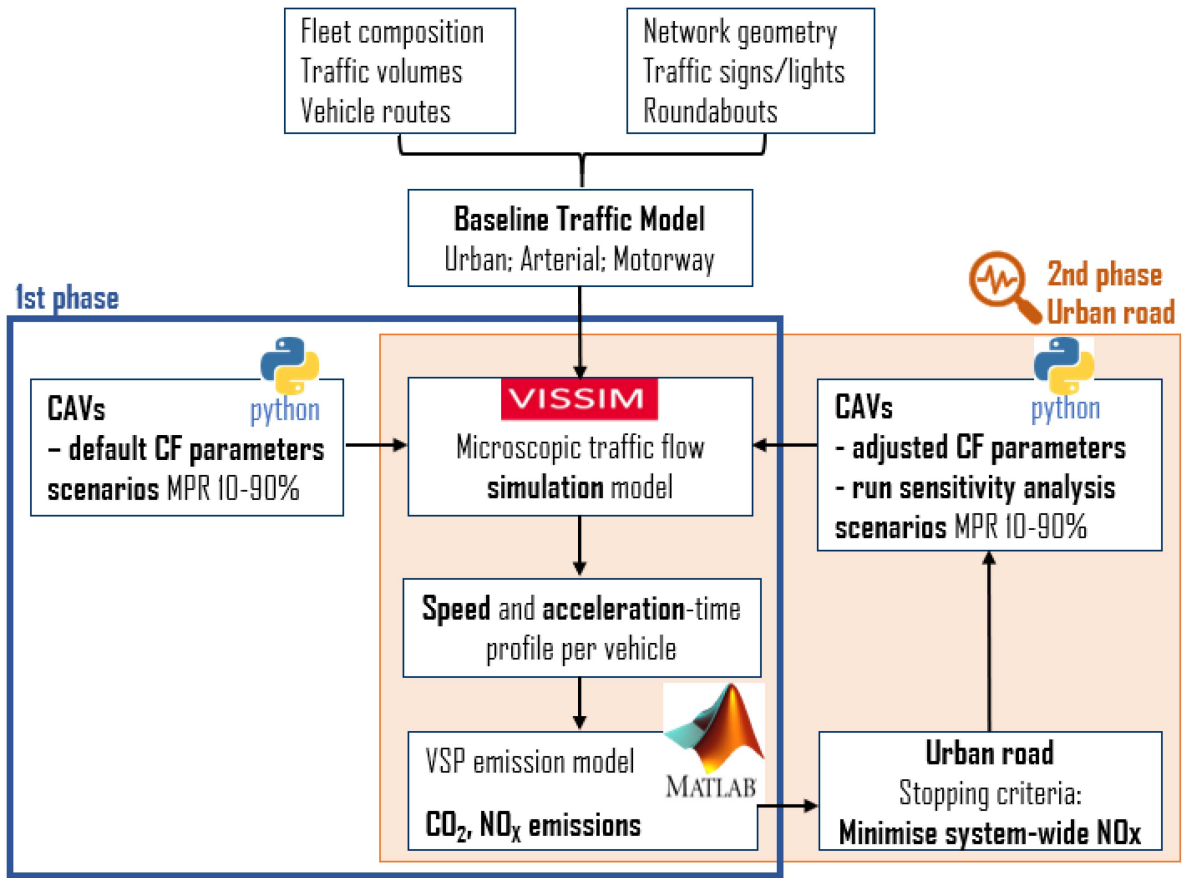
FIGURE 1. Methodology overview.

TABLE 1. Summary of the assumptions made in this work.

Parameter	Assumption
Demand	CAVs do not affect the matrix demand or vehicle occupancy rate
Street design	CAVs operate in mixed regime with CVs
Emission standards	CAVs have propulsion technology and emission standards similar to CVs
Automation and connectivity levels	V2V and V2I communications are not simulated. However, depending on the location, CAVs can adapt the speed to minimize emissions and adapt their driving behavior according to online hourly traffic demand information. Lateral behavior changes are not considered.
Human-driven interaction	CVs adapt to traffic conditions, but do not interact differently with CAV

as explained in Section III-A. CAVs are simulated by adopting the most relevant CFP drawn from the literature of reference [50], and local fleet composition is then changed on each scenario to assess different MPR of CAVs. The developed integrated platform extracts instantaneous speed and acceleration data for each vehicle in the network and then estimates the CO_2 and NOx emissions at the system level using the VSP methodology. The second phase involves a detailed microscopic analysis of a critical urban segment. This is done because the urban section yields a more complex network in terms of vehicle interaction profiles. Concretely, the urban segment under consideration can be regarded as a typical major road of a medium-sized city in terms of traffic conditions and infrastructures (1-2 lanes, traffic lights,

roundabout, vicinity of two schools, and residential and commercial areas). Thus, this urban segment is worthy of thorough investigation in terms of potential improvements in air quality. For that purpose, driving settings are tuned by following an exhaustive search procedure to perform a sensitivity analysis on the best combination set of parameters that leads to minimizing network-wide NOx emissions – a critical pollutant in core urban areas.

A. GENERAL ASSUMPTIONS
Some assumptions related to the demand, street design, emission standards, levels of automation and connectivity, and human-driven interaction were made throughout this research (Table 1).

1) DEMAND

Multiple MPR and changes in travel time-sensitivity have been shown to determine a wide range of effects on vehicle miles traveled from various CAV technologies [58], which can be shown to increase or decrease (e.g., [33]–[38]). Given this uncertainty and considering that this research aims to assess to which extent replacing CVs with CAVs brings potential environmental benefits due to the operational performance, the first study assumption is that the introduction of CAVs does not affect travel demand. Thus, the traffic volume on the network was considered fixed. Notice that this does not mean that the volumes on specific links are invariant on the simulation process. Congestion situations may occur due to the cautious behavior of CAVs, as it will be shown later.

2) ROAD DESIGN

Regarding road design, no dedicated lanes for CAVs are considered, so it is assumed that both CAVs and CVs will share the roads.

3) EMISSION STANDARDS

Following the recent work [43], it was considered that no significant differences were found in emissions per kilometer driven between CVs and CAVs with increased demand. This was further reinforced in a recent study based on emerging (although uncertain) propulsion technologies available in the market [36], [59]. Considering the objective of this paper and based on relevant literature (e.g., [12], [17], [50]), CAVs are assumed to have the same propulsion technology and emission standards as CVs. In fact, recent studies claim that in the decades to come, petroleum-based fueled vehicles will be prevalent (e.g., [60]). Despite some general perception that CAVs will be fully electric, some studies suggest the opposite (e.g., [59]). Moreover, vehicle electrification impact on the overall emissions is proportional to the share of vehicles being replaced with electric vehicles [17].

4) AUTOMATION AND CONNECTIVITY LEVELS

The core idea in this study is to explore the relative impacts of adjusting CFP of CAVs simulation on the network. Therefore, this work is not intended to provide an algorithm or control strategy for simulating CAVs, but to take advantage of existing traffic simulation platforms by tunning the complex car-following model's driving parameters. The first step relies on an analysis of the impact of CAVs introduction in the network by assuming a predefined driving behavior, regardless of the traffic environment. In a second step, it is assumed CAVs have information in terms of network environmental performance, and their driving behavior can be adjusted so that system-wide NOx emissions can be minimized. Nevertheless, it should be mentioned that vehicle to vehicle (V2V) and vehicle to infrastructure (V2I) communications are not explicitly simulated in terms of automation and connectivity levels, but cooperative behavior is implicit in the CFP chosen for modeling CAVs movements

or adjusting speed in the motorway section. In this case, CAVs-specific CFPs are tuned and further optimized, which means that CAVs should be capable of sensing the surrounding environment and need to have some sort of V2V and V2I communications. It should be mentioned that simulated CAVs are levels 3 or 4 [56] and can operate without further restrictions on the analyzed links. Concerning the lateral behavior, all simulated vehicles were set to occupy their desired position at free-flow conditions in the middle of lane [13], [61], and the default values of the VISSIM tool were adopted. Based on the case studies addressed in this research, the urban street has one lane by direction in almost its entire length. The road sections with two lanes represent dedicated lanes for left-turning only, being thus less influenced by the fact the CAVs have less aggressive, cautious or cooperative driving behaviors. Thus, considering these factors and the complexity of additional scenarios, tunning of the lane change and lateral parameters were excluded in the sensitivity analyses conducted here for CAVs optimization.

5) HUMAN-DRIVEN INTERACTION

Although it is out of the scope of this research to deeply analyze CVs reaction due to the operation of CAVs, the CVs (human-driven) driving behavior can be influenced by the surrounding vehicles movements, in particular, by the way CAVs operate. It should be clear that here, no specific control is used to tune CVs while interacting with CAVs: CVs can manage the operating actions based on the surrounding traffic environment.

B. TRAFFIC AND EMISSION MODELING

Due to the lack of real-world data, under simulated environment, CAVs driving settings can be adjusted using car-following models already implemented in traffic microsimulation platforms (e.g., [44], [50]). Such models involve various parameters related to the driving task as standstill distance, headway time, standstill acceleration, among others. Following previous works on exploring impacts of CAVs introduction ([23], [24], [45], [51], [54], [55], and more recently, [44]), the VISSIM traffic simulation software [13] is used in this study.

The VISSIM provides two versions of the Wiedemann car-following model for different application conditions [52]. It is commonly accepted to use the Wiedemann 74 model for urban traffic and merging areas, while the Wiedemann 99 is mostly used for freeway conditions. Moreover, the Wiedemann 99 is recommended to simulate CAVs due to the higher number of parameters available to modify and, therefore, more flexibility for adjustments to automated driving behavior [37], [50], [52].

Previous research [50], [51] investigated the best combination set of CFP for developing cautious and aggressive behaviors of CAVs so that GHG emissions would be minimized for urban and freeway segments. For that purpose, a sensitivity analysis through Monte Carlo

simulation and by modifying Wiedemann 99 parameters was performed [50], [51].

Despite the difficulty related to the lack of empirical data regarding the CAVs operation, the baseline scenario was rigorously calibrated and validated. The baseline scenario was validated in prior studies [62], involving typical calibration parameters (traffic, speed, and acceleration data) and VSP modes distribution between observed (gathered with Global Navigation Satellite System (GNSS) equipped vehicles) and modeled data. This validation process based on VSP distributions shows the capacity of the modeling platform to reproduce the dynamics of traffic flow correctly [62]. VSP is a proxy variable for engine load that is highly correlated with tailpipe emissions [62].

Here, it is proposed to simulate CAVs by adjusting CFP using a novel approach that consists in minimizing network-wide NOx emissions. The basic idea is that tunning driving behavior settings in CAVs will also affect other vehicle performances in the network. Based on relevant literature, the Wiedemann 74 car-following model was used to model CVs in the urban context, while the Wiedemann 99 model, which will capture the effects of various parameters, was used to simulate CVs in the rural and motorway segments, and CAVs in all road types ([13], [44], [50], [51]).

This research focuses on assessing the relative impact of CAVs on CVs over different link types. It is known that vehicle electrification is expected to bring emission benefits and that these can exceed the benefits presented by vehicle automation alone [50]. Furthermore, it was shown emission savings are proportional to the vehicles replaced as electric [17]; thus, here, CAVs were assumed to have similar propulsion technology and emission standards to CVs, as it is commonly accepted that individually owned autonomous vehicles would likely have the same per-vehicle-distance emissions as individually owned CVs [26]. However, the impacts in terms of local NOx emissions of a higher degree of electrification in the fleet can be easily adjusted to the respective percentage of electric vehicles in the fleet.

Regarding emission estimation, there exist various models in the literature, some based on engine operation and vehicle activity data [63]. They can be roughly divided into three classes: macroscopic, mesoscopic, and microscopic. Considering the purpose of the present study, a microscopic model was considered the best approach to better reflect the vehicle tailpipe emissions on a second-by-second basis. In particular, the Vehicle Specific Power - VSP methodology [64] was used in this study to estimate both CO_2 and NOx emissions, since it allows to compute the vehicle specific power (VSP [kW/ton]) based on the information on instantaneous speed ($v[m/s]$), acceleration ($a\ [m/s^2]$) and road grade (rg), that can be further used to estimate pollutant emissions with a reasonable level of detail. The VSP for a light-duty passenger vehicle can be given by (1):

$$VSP = v.\left[1.1a + 9.81.sin(arctan(rq))) + 0.132 + 0.00030v^3\right]$$

VSP values are assigned to 14 classes of required power (VSP modes), which in turn are associated with certain emission factors. For calibration purposes, the local fleet's emission rate was adapted as much as possible to the Portuguese vehicle fleet using five vehicles of different types [65]. Therefore, it was possible to estimate a modal average emission rate for each considered pollutant. Emission factors were organized over 14 VSP modes for Light-Duty Gasoline Vehicles (LDGV) with different engine sizes (1.4 – 2.2 L), Light Duty Diesel Vehicles (LDDV), and Light Commercial Vehicles (LCV) and HEV, as shown in Fig. 2.

CVs and CAVs emissions can be derived by segment based on the time spent in each VSP mode multiplied by the respective weighted average emission factor (WAEF) for each VSP mode (2):

$$E_P = \sum_{i=1}^{14} nVSP_i.WAEF_i$$

where E_p represents the total emissions (NOx or CO_2) generated in a given period; $nVSP_i$ is the time spent in each VSP mode (seconds), and $WAEF_i$ is the weighted average emission factors (g/second).

The VSP mode distributions of both CVs and CAVs were computed using speed and acceleration data from the traffic model. To improve the model's reliability and to determine statistical differences between VSP modes distributions among CVs and CAVs, the two-sample Kolmogorov–Smirnov (K–S) test at 95% confidence level was applied [66]. The two-sample K–S test is a well-known nonparametric method for comparing two data distributions, as it is sensitive to differences in both location and shape of the empirical cumulative distribution functions. The null hypothesis is that both samples have the same distribution. In this work context, the null hypothesis is that both CVs and CAVs VSP modes are drawn from the same distribution. Additionally, the two-sample K–S test is generally proposed when there is a natural ordering of the modes [67].

C. INTEGRATED PLATFORM

A combined MATLAB and Python platform was developed to work directly with VISSIM in an integrated way. In particular, the Python-based function was built to call VISSIM, set CFP for CAVs, and run a MATLAB routine developed in [68] to compute second-by-second pollutant emissions using the vehicle record data provided by VISSIM. Under this platform, the best combination of CFP for CAVs is obtained through a different combination-set based on adjusted values with a range limited by the values defined in [50], [51], and CoExist project [18]. The developed platform can provide CAVs driving settings that minimize network-wide NOx emissions, which is known to be a harmful human pollutant.

In the second phase of this research, the developed platform is used to conduct a thorough analysis of the
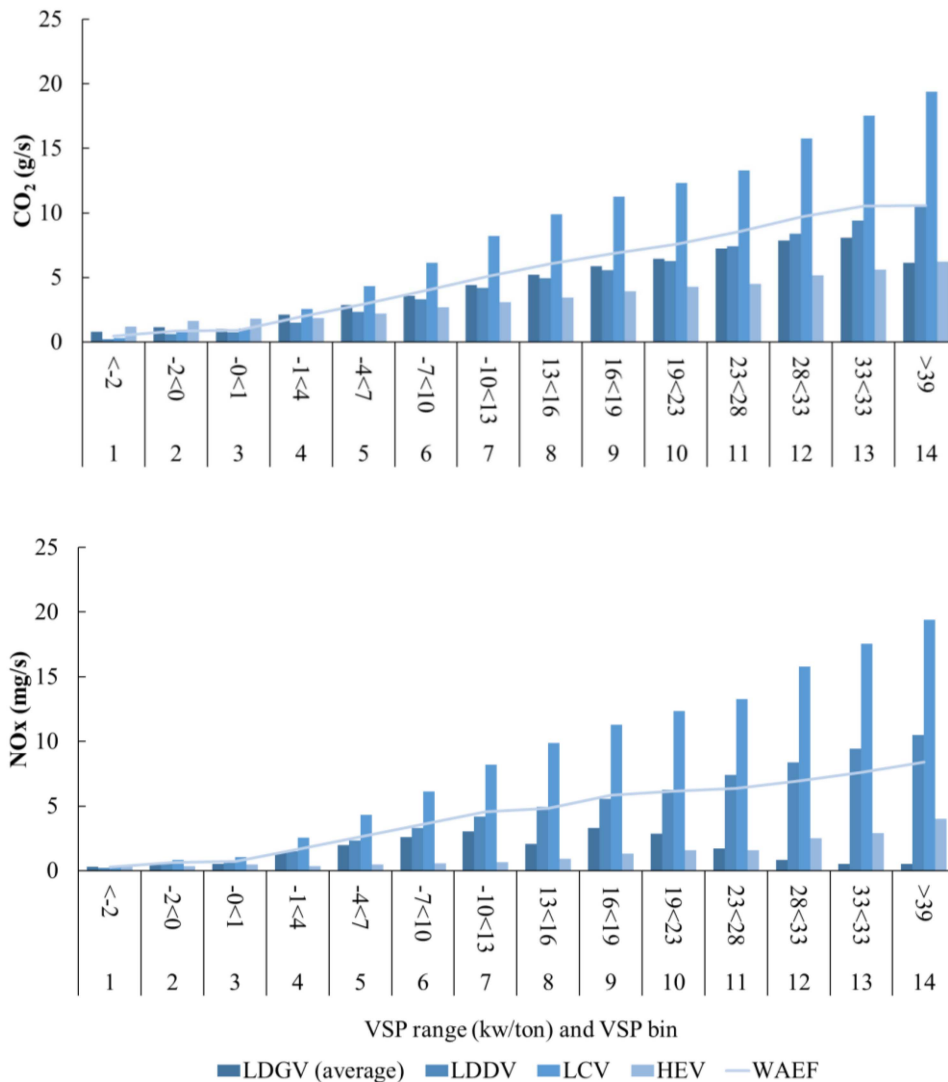
FIGURE 2. The weighted average (WAEF) and emission factors used to estimate emissions of a vehicle representative of the local fleet.

urban section. In this case, the analysis was extended to 24 hours to understand how CFP should vary throughout the day to allow for a reduction of the system-wide NOx emissions (which is conducted by considering different levels of traffic demand). This urban segment was selected because it involves a high rate of urbanization and nearby schools, which is likely to be a zone prone to join more people and increasing the risk of being exposed to air pollution.

As previously mentioned, the CC0, CC1, CC3, and CC8 parameters from the Wiedemann 99 car-following model were considered to be those that more significantly influenced the impacts on emissions ([50], [51]). Therefore, in the present research, several combination settings of these particular CFPs were generated based on [50], [51], while the remaining CFPs were set fixed. Concretely, 108 combinations were explored for the CC0, CC1, CC3, and CC8 parameters ($3 \times 4 \times 3 \times 3$), based on a grid of values ranging as defined in Table 2.

D. SCENARIO SET-UP
This study is intended to evaluate the impacts of CAVs introduction in different road segments. Five mobility scenarios representing different CAVs MPR were simulated, fixing the traffic demand, and considered that the CV traffic share is gradually replaced by automated vehicles. Thus, the share of CAVs in the overall network volume varies according to the following definition of scenarios: MPR 10%, MPR 30%, MPR 50%, MPR 70%, and MPR 90%. The baseline scenario (Baseline) corresponds to the current traffic context with 100% of CVs.

E. CASE STUDY
For exploring the potential impacts of CAVs penetration, the city of Aveiro (Portugal), was chosen for the experiments. The baseline traffic model was calibrated and validated using real CV data collected on different specific road segments of the study area, along 14 traffic monitoring points during the morning peak-hour (8.15–9.15 AM),

TABLE 2. CFP values explored in this paper.

CFP	Reference	National Road	Motorway (90 km/h)	Urban Avenue (adjusted)
CC0 [m]	1.50	1.47	0.50	(0.50; 1.50; 2.50)
CC1 [s]	0.90	1	1	(0.50; 0.90; 1.50; 2)
CC2 [m]	4	0	0	0
CC3 [s]	-8	-13.54	-4	(-4; -8; -16)
CC4 [m/s]	-0.35	-0.13	0.1	-0.10
CC5 [m/s]	0.35	0.13	0.1	0.10
CC6	11.44			0
CC7 [m/s^2]	0.25	0.08	0.45	0.05
CC8 [m/s^2]	3.50	3.72	3.90	(3.10;3.50; 3.90)
CC9 [m/s^2]	1.50	1.60	1.90	

(Sukennik, (2018) - CoExist project; Stogios, 2018)

TABLE 3. Summary of study segments to analyze the operational impact of CAVs (Bandeira *et al.*, 2018, Vicente *et al.*, 2018, IMT, 2019).

Segment	A	C	D
Road Type	Urban Avenue	National Road	Motorway
GPS Coordinates	40°38'20.1"N 8°39'01.0"W 40°38'03.7"N 8°38'38.4"W	40°37'25.27"N 8°39'1.39"W 40°39'19.43"N 8°37'5.41"W	40°38'49.43"N 8°36'46.84"W 40°38'22.87"N 8°39'51.17"W
Length [km]	0.75	4.5	5.1
Speed limit [kph]	40	70	120
# Lanes per direction	1-2	1 − 2	2
# TC	2 Traffic Lights Roundabout	8 Interchanges 1 three-lane Roundabout	2 Interchanges
Traffic [vph]	890 − 1 300	1440 − 2 100	1 560– 3 250
Built Environment	Residential and School	Retail Mixed land use	Residential and Nature

 # Number; TC − Traffic Control; vph − vehicles per hour

covering 550km. Both empirical monitoring and microscopic simulation of the baseline scenario were performed in earlier research [62], [69].

The selected area involves a network composed of different road types, each one with different traffic volumes and speed limits. This characteristic allows the model's ability to reproduce the impact of new types of vehicles, with different operational parameters optimized for different road types, on the performance of CVs. Table 3 summarizes relevant information for each road segment, including road type, GPS coordinates, length, number and traffic control treatment, and traffic volumes.

IV. RESULTS
In this section, the results of the proposed study are presented.

A. EFFECT OF CAVS ON VEHICLE SPECIFIC POWER DISTRIBUTIONS
The proportion of CAVs in the fleet and their operating behavior can influence traffic flow. Previous research showed that the relatively low share (less than 30% low-level automated vehicles) could have a limited effect than higher arbitrary penetration levels [70]. In this context and to assess to which extent the CAVs influence the dynamics of the vehicles operating on the network, in this section, we analyze the distribution of VSP bins for the various road segments, if the CAVs had a predefined configuration given by the CFP explored in [50], [51] (Table 2). Fig. 3 shows the cumulative profile of the VSP modal distribution of all vehicles operating for the different road segments. The presented profiles are for the scenario MPR 30% of CAVs for the morning peak-hour (similar trends are observed for scenarios of higher MPR of CAVs).

We first analyze the global baseline VSP distribution pattern on each route. As expected, the predominance of higher modes is notorious in the motorway section - A25 (only 10% occurrence of VSP modes lower than 5). On the urban road, reduced speed and stop-and-go situations are clear through the high frequency of lower VSP modes ranging between 1 and 4. Due to these traffic conditions, approximately 65% of
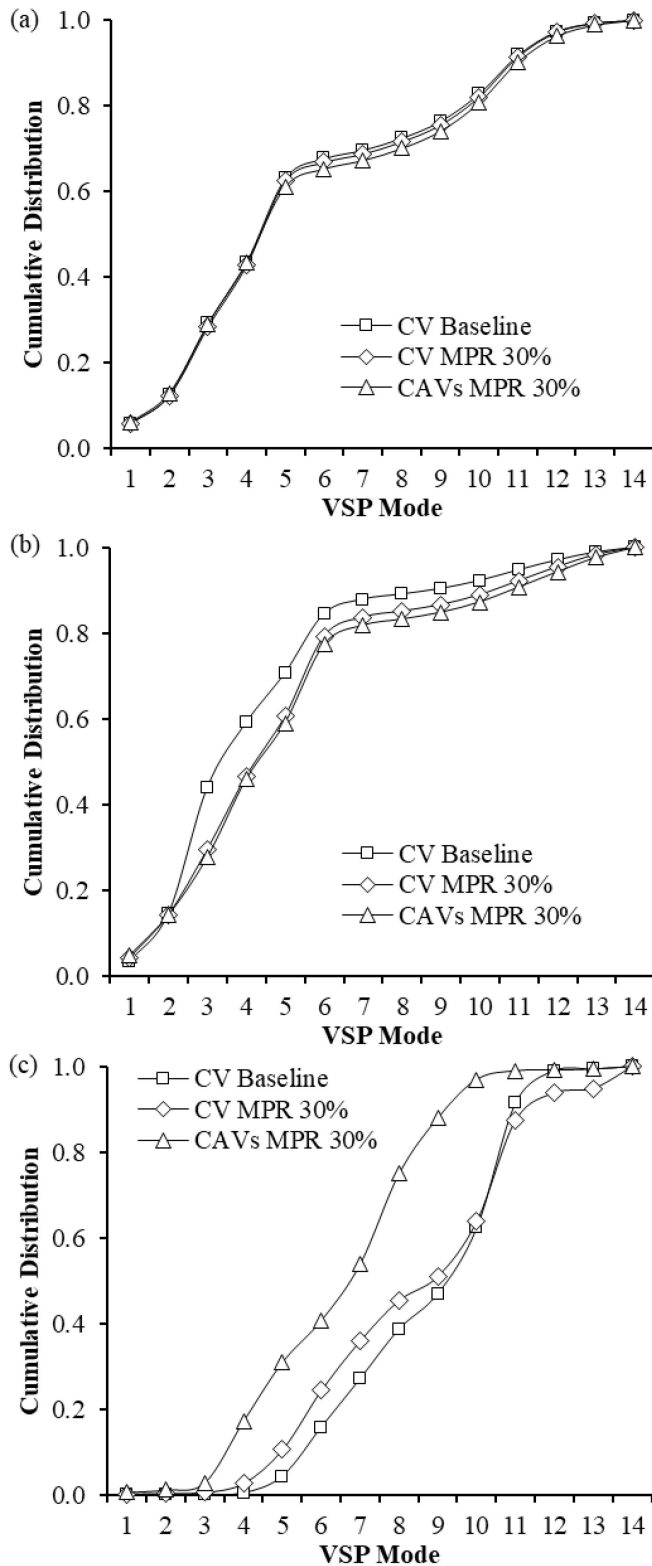
FIGURE 3. Cumulative profile of the VSP modal distribution of all vehicles operating for the different road segments: (a) urban; (b) rural; and (c) motorway.

the travel time is spent in VSP modes lower than 5. In the national road, it can be observed an intermediate VSP modal distribution and a higher prevalence of 5-7 VSP modes.

It should be mentioned that one can notice a difference in the dynamics translated into the different VSP modes profiles between CAVs and CVs in the various case studies.

Regarding the motorway section, it should be highlighted that the influence of varying the CFP without changing operational speed was tested in the first step. However, the low volume-to-capacity (V/C) ratio (between 0.21 and 0.43) and little interaction between vehicles lead to small impacts of changing car-following parameters. For this reason, the possibility of CAVs adjusting the speed to 90 km/h was simulated. Thus, it appears that in the Baseline scenario, CVs spent about 53% of the travel time in VSP modes greater than or equal to 9. Due to the new dynamics and speed limits imposed, in the MPR 30% scenario, CAVs only spend 12% of the time in VSP modes higher than 9. The influence of the presence of CAVs on the motorway also influences CVs' behavior. There is evidence of a smoother behavior with a greater predominance of intermediate modes. The two-sample K–S test at 95% confidence level showed no evidence that the two sets of data, i.e., CVs and CAVs, come from the same distribution for the MPR 30%. Moreover, there are also significant differences between VSP modes distribution for CVs before (Baseline) and after introducing 30% of CAVs in the network. In these cases, the maximal difference between the distribution (D–value) for this road segment were 0.37 (D-critical = 0.0020) and 0.0886 (D-critical = 0.0019), respectively.

In the national road, CVs and CAVs have different VSP distributions. Notably, the biggest difference between CVs' behavior before and after introducing 30% of CAVs is the frequency of VSP mode 3 movements associated with periods of congestion. In this type of road, the time spent in VSP mode 3 is reduced from 29% of the travel time to only about 15%. This reduction is balanced by the rise in modes 5 and 6, typically associated with moderate speeds or smooth accelerations. In the national road, D-values for VPS distribution comparison between CVs in the Baseline and CVs in MPR30 was 0.14 (D-critical = 0.0014). The distributions of VSP modes between CVs and CAVs for MPR 30% also differ statistically (D-Value 0.0192, D-critical = 0.0002).

Regarding CAVs introduction in the urban road, this impact is less clear. Comparing the VSP distribution of CVs and CAVs (MPR 30%), it can be observed that CAVs dynamics led to a slight reduction in CVs VSP modes 3 to 6 corresponding to moderate speeds and acceleration, and a slight increase in higher VSP modes, due to a more aggressive response of CVs to CAVs. Although the impact of CAVs is less evident in the urban segment, the distribution of VSP modes differs significantly at a 95% confidence level. The distributions of VSP modes between CVs in Baseline and MPR 30% has a D-Value of 0.00918 (D-critical = 0.0059), and under the MPR 30% scenario, such distributions of VSP modes for CVs and CAVs presented a D-Value of 0.0157 (D-critical = 0.0056).
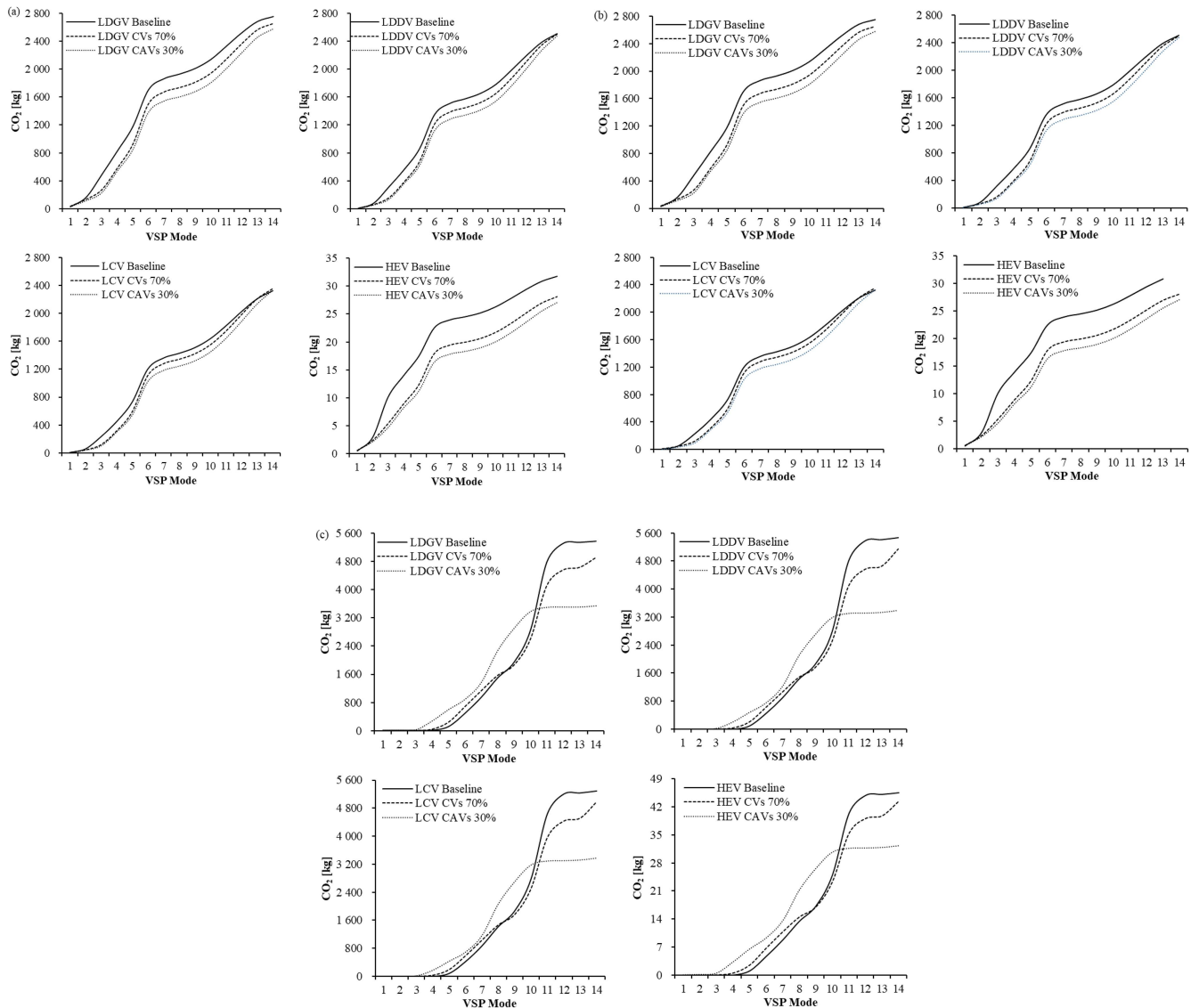
FIGURE 4. Cumulative CO₂ emissions over VSP modes for different vehicle categories for the Baseline and MPR 30% scenarios (a) urban; (b) national; and (c) motorway.

B. EFFECT OF CAVS ON VEHICLE DYNAMICS AND CATEGORY

In what follows, a brief analysis of the cumulative CO_2 emissions over VSP modes for different vehicle categories is presented for both the Baseline and the MPR 30 % scenarios.

From Fig. 4, in the case of the urban avenue, it can be observed the limited potential of CAVs to influence emissions. The slight observable changes result from more time spent in the higher modes due to restricted events of higher accelerations. This difference is most evident in light-duty and commercial diesel vehicles since the emission rate of CO_2 increases more sharply than for gasoline and hybrid cars with higher VSP modes.

On the national road, the impact of CAVs operation is more notorious. As a result of a slight increase in traffic performance, the major benefit is reducing the time spent in VSP mode 3, which is typically associated with stop-start situations. While in the Baseline more than 11% of CO_2

emissions are spent in VSP mode 3, this value is reduced to less than 5% in the MPR 30% scenario. However, increasing speed and reducing congestion have different effects. In fact, while in gasoline vehicles, this benefit is evident (reductions of up to 12%), but less advantageous in diesel vehicles. Indeed, for LCVs, the increase in speed leads to a marginal increase in CO_2 emissions. This consequence meets the expectation that diesel engines are more efficient than gasoline concerning fuel and CO_2, mainly at lower speeds.

A similar effect can be observed on the motorway, but due to an antagonistic role of CAVs. Due to the speed limitation, there is a significant transfer of time spent and CO_2 emissions in the higher modes than 10 for the moderate VSP modes, which exhibits higher emissions for 30% of CAVs than those of 70% of CVs. Within this framework, all vehicle classes benefited from the role of CAVs. However, in this situation, the diesel-powered CAVs would benefit most from

new traffic dynamics (38% reduction against 32 of LDGV). In addition, CVs would also benefit from traffic calming with reductions between 5-7%.

Considering the emissions factors used for characterizing the current fleet composition, it can be concluded that CAVs, as speed-moderating agents, tend to benefit mainly diesel vehicles. In turn, as agents that promote the performance of traffic flows, CAVs introduction would mainly benefit gasoline vehicles.

C. EMISSIONS PER VEHICLE AND RELATIVE CHANGE FOR DIFFERENT MPR

An overview of emissions per vehicle, per unit of distance, in each of the different road types, considering all vehicles (CAVs and CVs), is depicted in Fig. 5. These plots represent the variability of the 10 run random seeds' results according to the model stochasticity [71]. It can be observed that in the sections with traffic singularities (e.g., traffic lights and roundabouts), which is the case of the urban road, the variability of standard deviation is higher, with the coefficient of variation for CO_2 above 62% and NOx greater than 30%.

The Baseline represents the current traffic scenario. In any of the analyzed sections, the CAV gradual introduction led to changes in the pollutant emission levels for any other scenario. In the urban avenue, higher pollutant emissions are observed (>200g/km CO_2), mainly due to traffic lights, thus, leading to some congestion and stop-and-go situations. In this road type, increasing the CAVs MPR in the network also increases pollutant emissions up to 4% CO_2 and 14% NOx using the CFP suggested in the literature for CAVs [51]. A detailed analysis of the simulation has shown that two factors have contributed to this increase. First, a slight increase in traffic demand and traffic volumes (1 to 2%) is observed during the simulation period, resulting from the rise in the flow capacity of the intersections upstream of this section (faster response times of CAVs). Second, and more importantly, the effect of operational parameters is very relevant for these results, particularly the increase in CC8 (see Table 2), which corresponds to the acceleration after a stop to the cruising speed. This change leads to more aggressive accelerations of CAVs than CVs without being offset by a corresponding effect on the traffic performance offered by other parameters such as the standstill distance (CC1). Moreover, the national road yields the lowest average emissions. In this case, significant emission reductions are obtained along with the increase in CAVs MPR. Specifically, reductions between 11 and 18% for CO_2 and 10 and 16% for NOx were observed. In this context, the CFP assigned to CAVs and based on [50], [51] seem to be more appropriate to this road section. Fig. 5 confirms there is a significant effect on emissions reduction in line with the growing MPR of CAVs (3 to 18% for CO_2; and 4 to 32% for NOx).

Fig. 6 shows the relative difference in CO_2 and NOx emissions for CAVs, CVs, and total fleet compared to Baseline emissions. For almost all MPR scenarios, CVs emissions

are affected by the presence of CAVs. The effect tends to be environmentally positive in motorway sections, while in the urban section, CAVs operation is environmentally counterproductive. Interestingly, at the urban level, the magnitude of emission changes on CVs is higher in scenarios of greater balance between CAVs and CVs, particularly MPR 30% (30%-70%) and MPR 50% (50%-50%). This degree of impact results from a higher interaction of vehicles with different dynamics. These interactions lead to more acceleration events and, consequently, higher NOx emissions. In the motorway and national road sections, a linear relationship between the percentage of CAVs and the effect on the reduction of CVs emissions was found (coefficient of determination, R^2, of 90%), as shown in Fig. 6. Hence, if more CAVs circulate at optimized speeds, such as in motorways, this will lead to a better influence from the environmental perspective, which seems consistent with the literature [50].

D. COOPERATIVE CAVS FOR REDUCING NOX UNDER DIFFERENT TRAFFIC SCENARIOS AND MPR – URBAN AVENUE

Considering the negative effects of CAVs previously reported on the urban road and the relevance of improving air quality levels in an area of high vulnerability (presence of schools and high population density), a thorough analysis was conducted for this road. In this second phase, the core idea was to evaluate to what extent a tuning in the driving parameters would make it possible to reduce the emissions of a critical local pollutant such as NOx over 24 hours. For this purpose, as previously mentioned, a sensitivity analysis was performed based on the results from [15], [37], where 108 combinations of the CFPs (CC0, CC1, CC3, and CC8) used to emulate CAVs driving behavior were explored. Fig. 7 exhibits the hourly emissions produced and the relative variation achieved for each hour, through an exhaustive search for adjusting the key CFP parameters that minimize system NOx emissions for four different demand periods: i) Extremely reduced demand overnight, ii) Daytime average demand; iii) Evening Rush Hour; iv) Reduced demand (Early night).

During the night period (1h-8h), with very low demand, the impact of the CAVs contribution to emissions change is rather small. However, as demand increases, the contribution of CAVs for the reduction of network-wide NOx emissions also increases, reaching the maximum value between 14h and 15h during a relative peak of moderate demand. In this period, with the volume-to-capacity (V/C) ratio between 0.75 and 0.80, reductions between 12 and 23% were observed. During the maximum peak-period (17h-19h), there is also a considerable reduction in emissions (up to 15%). Although sensitivity analysis is focused on a tighter period, the fact that the network is close to saturation limits the potential of CAVs to reduce NOx emissions, with the V/C ratio reaching an approximate value of 1.03 at peak-time.
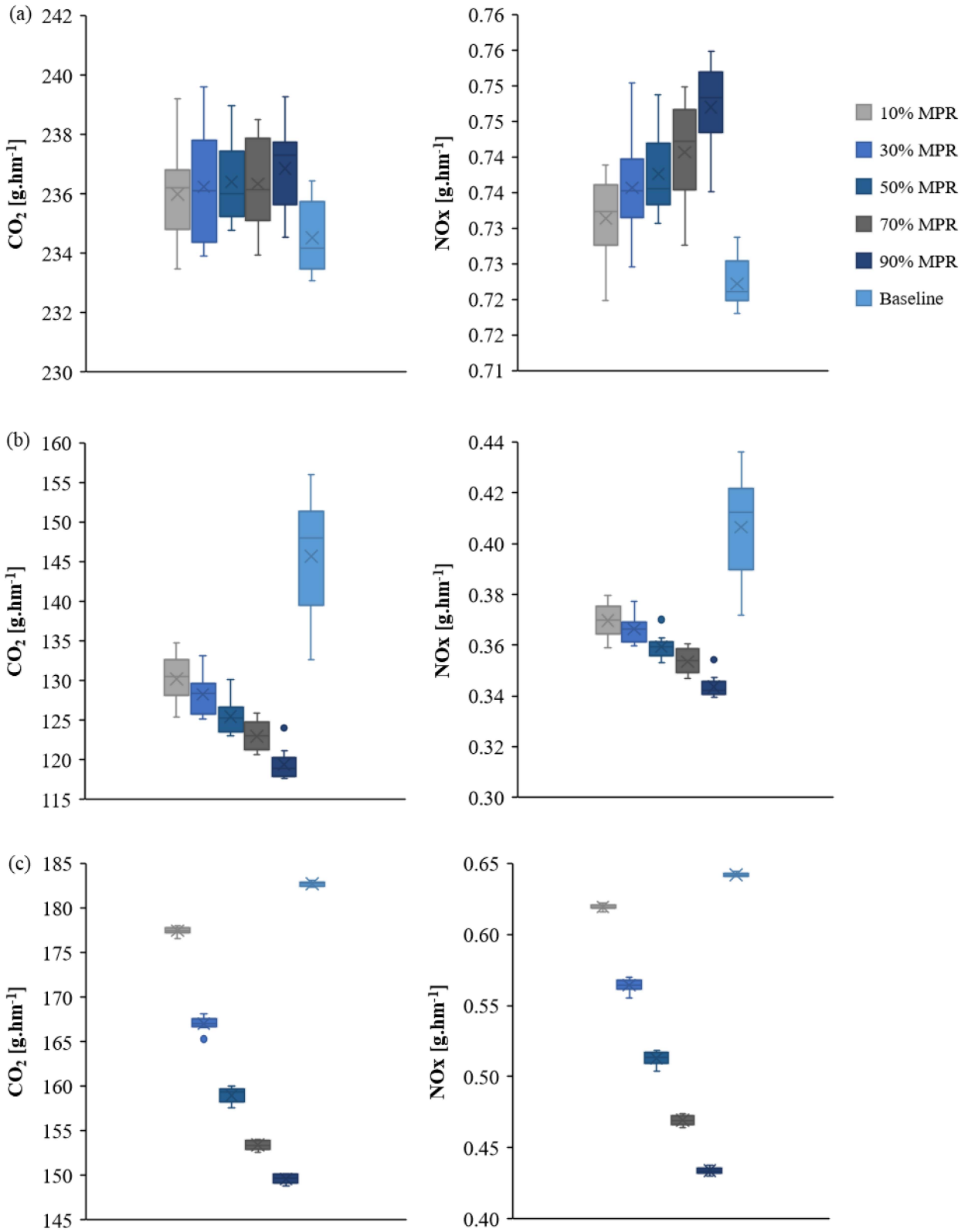
FIGURE 5. Average CO_2 and NOx emission factors (g/km) per vehicle for the Baseline and different MPR scenarios and on different road types (a) urban; (b) national; and (c) motorway.

In terms of daily emission reductions, the major relative contribution of CAVs to reduce system NOx emissions is between the Baseline and the MPR 10%, with a 2% reduction. Then, the impact of CAVs on emissions savings concerning the previous scenario is progressively less effective. The minimum impact (1%)
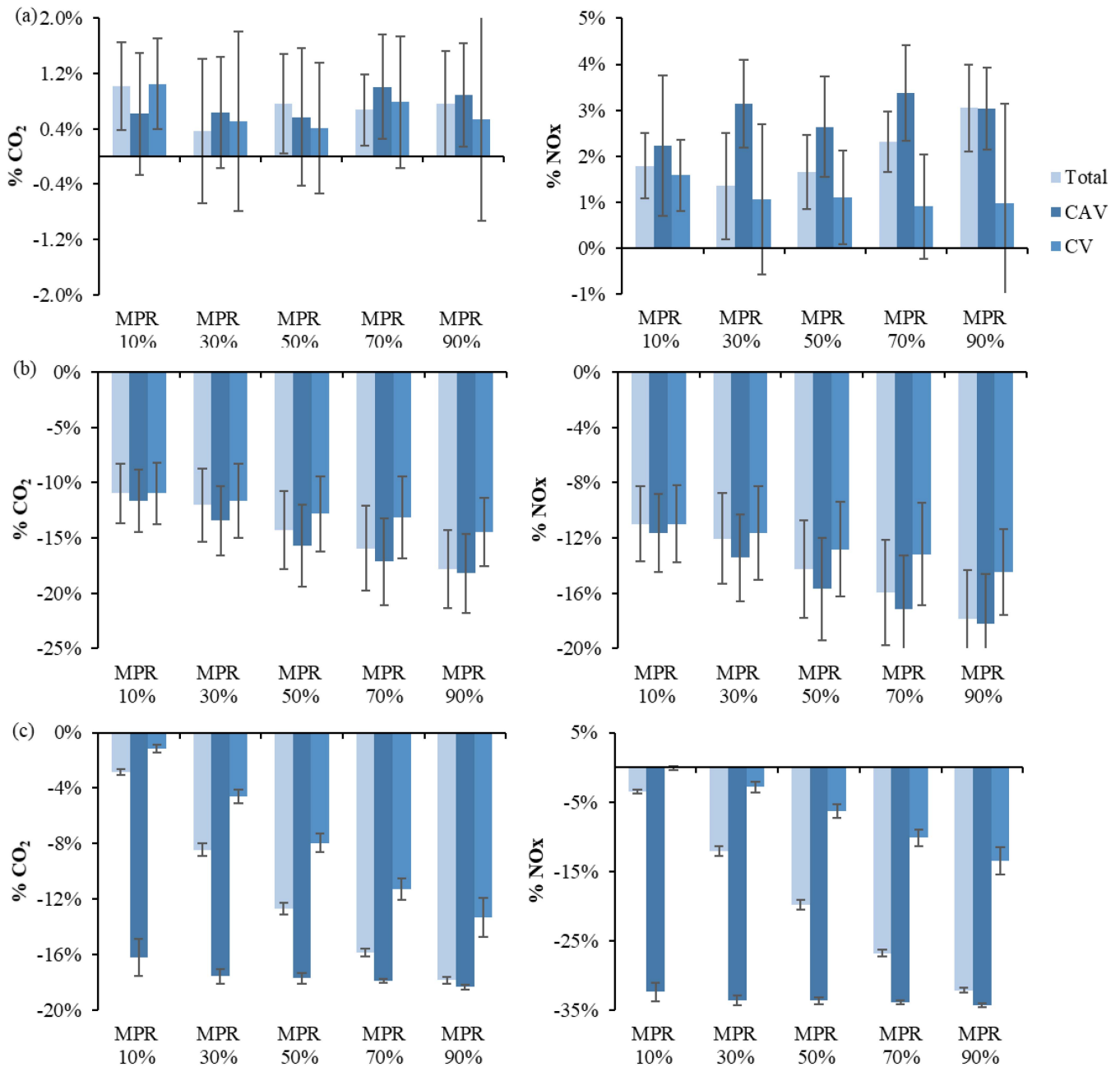
FIGURE 6. Comparison of the total CO_2 and NOx emissions of CAVs and CVs over multiple MPR in relation to Baseline for (a) urban; (b) national; and (c) motorway.

is observed between the MPR 70% and MPR 90% scenarios, as shown in Fig. 8. This difference is explained by the fact that CVs tend to adapt to the driving dynamics of CAVs as they become dominant in the network.

Fig. 9 displays that for all MPR scenarios and the various periods of congestion, CC8 tends to be higher (3.9 m/s²) in the daily periods of greater congestion and lower (3.1 m/s²) in the night periods of very low demand.

A NOx reduction trend was found with the increase of the CC8 parameter (standstill acceleration) during particular day periods. This finding is not self-evident, as we

might expect that NOx emissions increase when the engine is under load instance, during fast acceleration. This effect can be justified by the decrease in congestion levels and less time emitting pollution by the joint fleet of CAVs and CVs. These results are consistent with the previous studies showing that eco-driving strategies based on slower speeds and smother accelerations may increase traffic congestion at the road network or vehicle fleet level and likely increase emissions [72], [73]. In the absence of congestion, the claimed environmental benefits of smoother acceleration for CAVs would positively impact the fleet level (CV + CAVs) in line with [74].
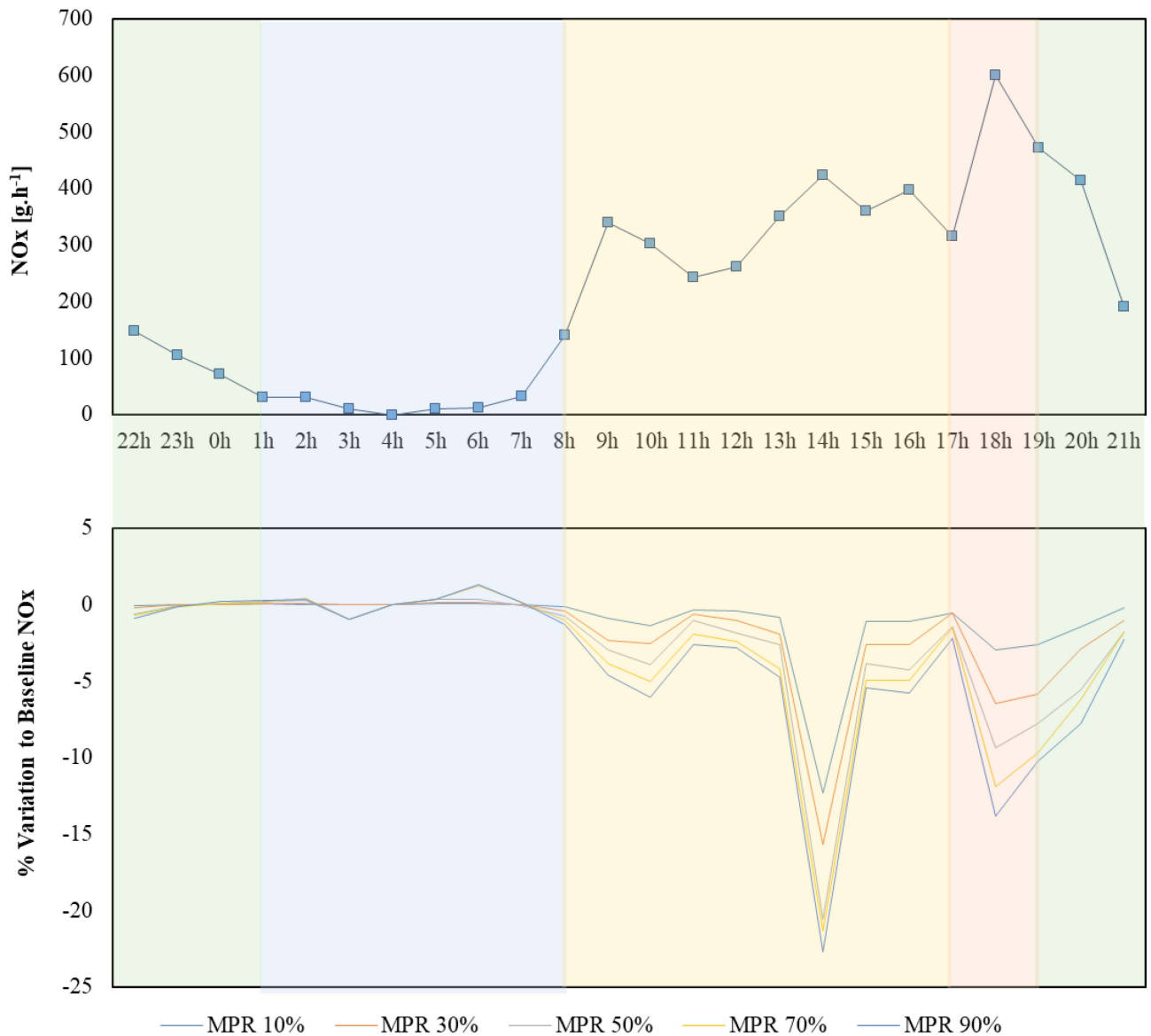
**FIGURE 7.** Comparison of NOx for 24 hours, by scenario.

Following the obtained results, evidence for the 24-hour period shows that CC0 and CC1 parameters are similar, assuming the minimum values (0.5). These values are in line with the work [24], indicating that these parameters should be reduced to 0.38 and 0.45, respectively, to improve traffic performance. However, it should be taken into account that, in the first stage, this fine-tuning of values may not be immediately attainable. This scenario would imply that CAVs had a deep awareness of traffic context, allowing smaller gaps for all maneuvers. Regarding the remaining factors, CC3 frequently oscillates for the various simulations with no evident relationship to congestion and MPR levels.

In terms of total travel time, CAVs operation impacts are globally positive, with the largest reductions occurring at rush hour (up to 2.4%) and marginal increases (<1%) over the night period, as shown in Fig. 10.

E. DISCUSSION AND STUDY LIMITATIONS
All the results previously presented must be considered in light of the assumptions made and the limitations of the methodological approach.

The first aspect is related to the simulation approach of this work. Although a considerable body of research considers that adapting Wiedemann parameters can be a valid approach to simulating CAVs (e.g., [24], [44], [50], [51], [52]), this approach poses some limitations, since the output of simulation model is completely dependent on the selected CFPs. Bearing in mind that validation of any new modeling approach would also be hindered due to the lack of empirical data, new models capturing the complexity of the interactions between CVs and CAVs can be integrated into future research. For instance, Calvert and Arem [75] demonstrated that simulating longitudinal driving behavior of automated
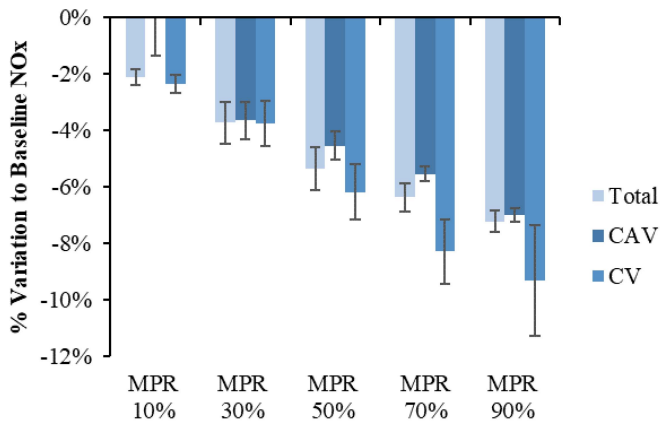
FIGURE 8. Comparison between the total NOx emissions over multiple MPR in relation to Baseline.

vehicles may be straightforward; but modeling the response of human drivers to CAVs is much more difficult. Some novel approaches explicitly considering driver cognitive loading and related performance with CAVs have been recently developed [75]. The integration of similar tools may improve how the interactive effects between CVs and CAVs are considered. It should be highlighted that even without considering the introduction of CAVs, previous studies based on naturalistic data indicate that the drivers exhibit different behaviors depending upon the speed, implying an increase in aggression at certain vehicle speeds.

Another limitation is related to the fact that the influence of CAVs lateral movement was not explored. Nevertheless, in this case study (low V/C ratio or lanes with specific turn purposes), this effect can be considered less important. Moreover, each scenario assumed the CAVs would have a similar behavior based on a predefined driving behavior configuration or assuming a homogenous reaction of CAVs to traffic contexts in the urban avenue case study. Evolution of technology will be made progressively through cruise control commands that are merely auxiliary or informative supporting systems in the initial stages; then a growing market share of fully autonomous systems may be expected.

One of the challenges of research on CAVs is to consider the heterogeneity of human behavior and technological advancement, without compromising the efficiency in optimizing and identifying key variables. Despite the uncertainty and assumptions behind the present work, we consider that this study can address the main research questions. On the one hand, it has been shown that introducing a subpopulation of CAVs with new plausible dynamics behavior can (positively or negatively) affect the dynamics and pollutant emissions of the remaining vehicles in the road traffic system. On the other hand, it was demonstrated this effect changes for different road types, and if the policy objective is to maximize CAVs environmental benefit, it will be vital to anticipate ad-hoc strategies for different road types and traffic demand contexts.

V. CONCLUSION

CAVs are expected to reshape future transport networks. This paper presents an effort to explore the environmental impacts of CAVs gradual introduction by considering road types with different characteristics, such as different speed limits and traffic volumes. A simulation-based framework is suggested to take advantage of existing traffic simulation platforms. In the first phase, CAVs were assumed to have a predetermined fixed behavior based on driving parameters found in the literature; in the second phase, new forms of cooperative behavior were explored by adjusting CAVs driving settings. For the first time, the optimal set of CFP for emulating CAVs that allow a network-wide minimization of NOx emissions was explored. Five scenarios of CAVs MPR were considered. The developed integrated platform combines traffic simulation and CO_2 and NOx emission estimation. A detailed analysis of the distribution of VSP modes has shown that CAVs have the potential to adapt their operating behavior and affect the dynamics of the surrounded vehicles to minimize a given environmental impact at a network scale. However, the magnitude of these impacts varies according to the type of road, demand, and CAVs MPR. Concretely, the main contributions of this work are threefold: 1) analyzing the distributions of accelerations and VSP modes between CVs and CAVs on different types of roads; 2) understanding the differences in terms of CAVs MPR in emissions and VSP distributions; and 3) optimization of the parameters of the CAVs taking into account the type of road, so that network-wide emissions are minimized.

A network composed of three different road types, namely, urban, rural, and motorway segments, was considered for the case study. These case studies were chosen mainly due to their differences regarding singularities, speed limits, and traffic volumes. The findings allowed us to clearly address the main research questions and to draw the following conclusions:

1) Considering the reference values of driving behavior found in the literature, the impact of the introduction of CAVs on emissions widely varied among different road types. CAVs were shown to be particularly beneficial for the environment in the national road, with emission reductions up to 10%. By contrast, in the urban corridor, impacts were shown to be detrimental. At the motorway level, with a low V/C ratio, the impacts are also negligible. Nevertheless, optimizing the speed to 90 km/h allows reductions up to 18% of CO_2 and 32% of NOx.

2) In sections outside the urban context, the environmental impacts resulting from the presence of CAVs are positive, following a strong linear relationship with higher MPR. In the urban sections, the most negative impacts are observed for MPR 30% and MPR 50%. For these MPRs, total CO_2 and NOx emissions increased up to 4% and 8% in the urban avenue, respectively.

3) CAVs showed to significantly influence the environmental performance of CVs with possible savings ranging from 3 up to 13%. Assuming that an electric engine does
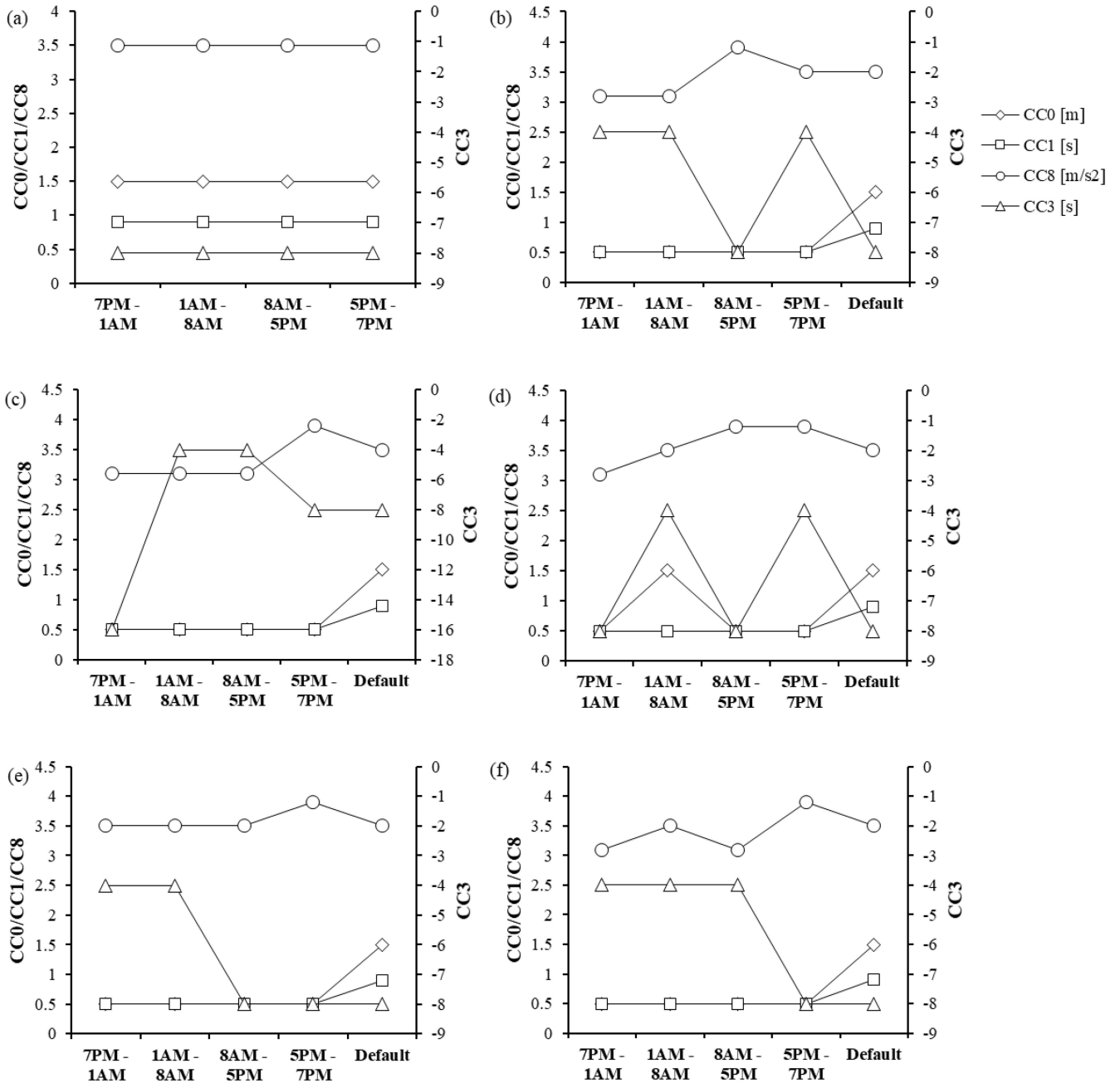
FIGURE 9. CFP for different MPR: (a) Baseline; (b) MPR 10%; (c) MPR 30%; (d) MPR 50%; (e) MPR 70%; (f) MPR 90%.

not significantly affect the explored CFP to simulate CAVs operating behavior, these results suggest that even considering that CAVs could be predominantly fully electric in the near future, the impact of their movements on surrounded vehicles and on network-wide emissions should be considered and adjusted to different driving scenarios.

4) If an ad-hoc exhaustive search procedure is performed considering the type of road, traffic demand, and CAVs MPR, CAVs operation's impact can yield promising benefits at network scale (less total NOx emissions between 15 and 23%, depending on the MPR of CAVs).

5) Results suggest CAVs should adopt more aggressive behavior in higher volumes time-periods, and smoother behavior in the remaining periods to maximize the benefits in terms of network-wide NOx emissions.

The findings are valuable to policymakers and vehicle manufacturers since they can provide insights into the possible benefits and impacts of CAVs in pollutant emissions while sharing the roads with CVs. Significant system emissions can be achieved by just tuning the driving behavior parameters to optimized values such that network-wide emissions are minimal.
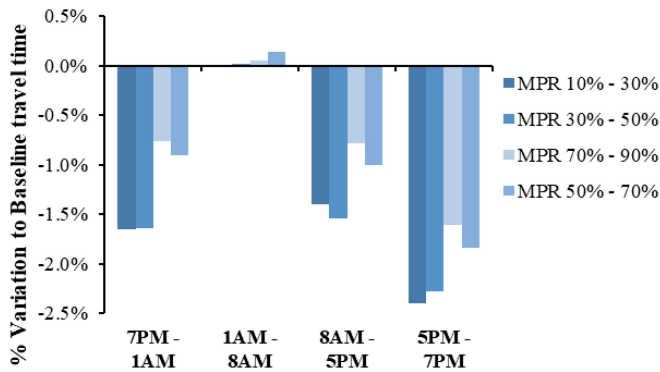
FIGURE 10. Comparison of travel times in different scenarios.

Realistically, the dynamic variation of the CAVs driving parameters on a large scale will certainly not be easily feasible in an initial context of poor connectivity and cooperation between the infrastructure and the vehicles that make it possible, for example, to adjust the parameters for more aggressive configuration over higher congestion levels. However, the encouraging insights of this work point to research directions. For instance, at least in pilot studies, or in highly vulnerable links (e.g., high levels of population exposure, or hotspots in terms of polluted areas), CAVs could adjust their behavior to minimize specific environmental problems. Since it is not clear the effect of CAVs introduction on traffic demand, more simulation scenarios should be conducted. Future research will focus on developing a multi-objective optimization model with decision variables in the form of the CFP that should be optimized for different links, considering different saturation levels and emission standard scenarios, and air quality impacts. In addition to NOx and CO_2, other pollutants such as PM, and other traffic-related externalities such as road accidents, must be considered. It is also in mind further improvement to account for different roads' singularities by allowing driving behavior settings to be adjusted dynamically and adaptively.

In light of the methodological limitations associated with modifying the parameters of the car-following model to represent the behavior of the CAVs in a mixed traffic environment, future research should explore alternative driving logics algorithms, and investigate heterogeneous human behavior categories and its reaction to CAVs over different traffic contexts and road types.

REFERENCES

[1] *Statistical Pocketbook*, Eur. Comm., Brussels, Belgium, 2020.
[2] European Commission. (Apr. 2018). *Transport in the European Union—Current Trends and Issues*. [Online]. Available: https://ec.europa.eu/transport/sites/transport/files/2018-transport-in-the-eu-current-trends-and-issues.pdf
[3] *Growing Preference for SUVs Challenges Emissions Reductions in Passenger Car Market*, Int. Energy Agency, Paris, France, 2019.
[4] *Average CO2 Emissions From New Carsand New Vans Increased Again in 2019*, Eur. Econ. Area, Copenhagen, Denmark, 2019.
[5] A. Krajinska, *A New Dieselgate in the Making*, Transp. Environ., Brussels, Belgium, 2020.

[6] P. Fernandes, R. Tomás, E. Ferreira, B. Bahmankhah, and M. C. Coelho, "Driving aggressiveness in hybrid electric vehicles: Assessing the impact of driving volatility on emission rates," *Appl. Energy*, vol. 284, Feb. 2021, Art. no. 116250, doi: 10.1016/j.apenergy.2020.116250.
[7] S. C. Anenberg et al., "Impacts and mitigation of excess diesel-related NOx emissions in 11 major vehicle markets," *Nature*, vol. 545, pp. 467–471, May 2017, doi: 10.1038/nature22086.
[8] G. H. de A. Correia and B. van Arem, "Estimating urban mobility patterns under a scenario of automated driving: Results from a model application to Delft, The Netherlands," in *Proc. 96th Annu. Transp. Res. Board Meeting*, 2017, p. 20.
[9] Q. Lu, T. Tettamanti, D. Hörcher, and I. Varga, "The impact of autonomous vehicles on urban traffic network capacity: An experimental analysis by microscopic traffic simulation," *Transp. Lett.*, vol. 12, no. 8, pp. 540–549, 2020, doi: 10.1080/19427867.2019.1662561.
[10] P. A. Hancock, I. Nourbakhsh, and J. Stewart, "On the future of transportation in an era of automated and autonomous vehicles," *Proc. Nat. Acad. Sci.*, vol. 116, no. 16, pp. 7684–7691, Apr. 2019, doi: 10.1073/pnas.1805770115.
[11] A. Talebpour and H. S. Mahmassani, "Influence of connected and autonomous vehicles on traffic flow stability and throughput," *Transp. Res. Part C, Emerg. Technol.*, vol. 71, pp. 143–163, Oct. 2016, doi: 10.1016/j.trc.2016.07.007.
[12] J. Conlon and J. Lin, "Greenhouse gas emission impact of autonomous vehicle introduction in an urban network," *Transp. Res. Rec.*, vol. 2673, no. 5, pp. 142–152, 2019, doi: 10.1177/0361198119839970.
[13] *PTV VISSIM 9 User Manual*, Planung Transp. Verkehr, Karlsruhe, Germany, 2016.
[14] V. Milanés, S. E. Shladover, J. Spring, C. Nowakowski, H. Kawazoe, and M. Nakamura, "Cooperative adaptive cruise control in real traffic situations," *IEEE Trans. Intell. Transp. Syst.*, vol. 15, no. 1, pp. 296–305, Feb. 2014, doi: 10.1109/TITS.2013.2278494.
[15] V. L. Knoop, M. Wang, I. Wilmink, D. M. Hoedemaeker, M. Maaskant, and E.-J. Van der Meer, "Platoon of SAE level-2 automated vehicles on public roads: Setup, traffic interactions, and stability," *Transp. Res. Rec. J. Transp. Res. Board*, vol. 2673, no. 9, pp. 311–322, Sep. 2019, doi: 10.1177/0361198119845885.
[16] Y. Rahmati, M. K. Hosseini, A. Talebpour, B. Swain, and C. Nelson, "Influence of autonomous vehicles on car-following behavior of human drivers," *Transp. Res. Rec.*, vol. 2673, no. 12, pp. 367–379, Dec. 2019, doi: 10.1177/0361198119862628.
[17] R. E. Stern et al., "Quantifying air quality benefits resulting from few autonomous vehicles stabilizing traffic," *Transp. Res. D, Transp. Environ.*, vol. 67, pp. 351–365, Feb. 2019, doi: 10.1016/j.trd.2018.12.008.
[18] P. Sukennik. (2018). *Micro-Simulation Guide for Automated Vehicles—CoExist Project*. [Online]. Available: https://www.h2020-coexist.eu
[19] M. Kamrani, R. Arvin, and A. J. Khattak, "Extracting useful information from basic safety message data: An empirical study of driving volatility measures and crash frequency at intersections," *Transp. Res. Rec. J. Transp. Res. Board*, vol. 2672, no. 38, pp. 290–301, Dec. 2018, doi: 10.1177/0361198118773869.
[20] I. Mahdinia, R. Arvin, A. J. Khattak, and A. Ghiasi, "Safety, energy, and emissions impacts of adaptive cruise control and cooperative adaptive cruise control," *Transp. Res. Rec.*, vol. 2674, no. 6, pp. 253–267, Jun. 2020, doi: 10.1177/0361198120918572.
[21] R. Arvin, A. J. Khattak, M. Kamrani, and J. Rio-Torres, "Safety evaluation of connected and automated vehicles in mixed traffic with conventional vehicles at intersections," *J. Intell. Transp. Syst. Technol. Plan. Oper.*, vol. 25, no. 2, pp. 170–187, 2021, doi: 10.1080/15472450.2020.1834392.
[22] B. Friedrich, "The effect of autonomous vehicles on traffic," in *Autonomous Driving*, M. Maurer, J. Gerdes, B. Lenz, and H. Winner, Eds. Berlin, Germany: Springer, 2016, pp. 317–334, doi: 10.1007/978-3-662-48847-8_16.
[23] S. Lee, E. Jeong, M. Oh, and C. Oh, "Driving aggressiveness management policy to enhance the performance of mixed traffic conditions in automated driving environments," *Transp. Res. A, Policy Pract.*, vol. 121, pp. 136–146, Mar. 2019, doi: 10.1016/j.tra.2019.01.010.
[24] A. Rezaei and B. Caulfield, "Simulating a transition to autonomous mobility," *Simulat. Model. Pract. Theory*, vol. 106, Jan. 2021, Art. no. 102175, doi: 10.1016/j.simpat.2020.102175.

[25] S. Rafael *et al.*, "Autonomous vehicles opportunities for cities air quality," *Sci. Total Environ.*, vol. 712, Apr. 2020, Art. no. 136546, doi: 10.1016/j.scitotenv.2020.136546.

[26] J. M. Greenwald and A. Kornhauser, "It's up to us: Policies to improve climate outcomes from automated vehicles," *Energy Policy*, vol. 127, pp. 445–451, Apr. 2019, doi: 10.1016/j.enpol.2018.12.017.

[27] M. Bertoncello and D. Wee, *Ten Ways Autonomous Driving Could Redefine the Automotive World*, McKinsey, New York, NY, USA, 2015.

[28] J. Anderson, N. Kalra, K. Stanley, P. Sorensen, C. Samaras, and O. Oluwatola, *Autonomous Vehicle Technology: A Guide for Policymakers*, RAND Corp., Santa Monica, CA, USA, 2016.

[29] J. Liu, K. Kockelman, and A. Nichols, "Anticipating the emissions impacts of autonomous vehicles using the MOVES model" in *Proc. 95th Trans. Res. Board Annu. Meeting*, Washington, DC, USA, 2017. [Online]. Available: https://scholar.google.com/scholar?cluster=16738901287795133315&hl=pt-PT&as_sdt=0,5

[30] J. Conlon, S. Ballare, and J. Lin, "Analysis of environmental impacts of autonomous vehicles," in *Proc. 97th Annu. Transp. Res. Board Meeting*, 2018, p. 10.

[31] M. Guériau, R. Billot, N.-E. El Faouzi, and J. Monteil, "Contribution to the assessment methodology for connected and automated vehicles on traffic," in *Proc. 97th Annu. Transp. Res. Board Meeting*, 2018, p. 19.

[32] Z. V. Laan and K. F. Sadabadi, "Operational performance of a congested corridor with lanes dedicated to autonomous vehicle traffic," *Int. J. Transp. Sci. Technol.*, vol. 6, no. 1, pp. 42–52, Jun. 2017, doi: 10.1016/j.ijtst.2017.05.006.

[33] C. D. Harper, C. T. Hendrickson, S. Mangones, and C. Samaras, "Estimating potential increases in travel with autonomous vehicles for the non-driving, elderly and people with travel-restrictive medical conditions," *Transp. Res. C, Emerg. Technol.*, vol. 72, pp. 1–9, Nov. 2016, doi: 10.1016/j.trc.2016.09.003.

[34] E. H. Nemoto, R. Issaoui, D. Korbee, I. Jaroudi, and G. Fournier, "How to measure the impacts of shared automated electric vehicles on urban mobility," *Transp. Res. D, Transp. Environ.*, vol. 93, Apr. 2021, Art. no. 102766, doi: 10.1016/j.trd.2021.102766.

[35] S. Puylaert, M. Snelder, R. van Nes, and B. van Arem, "Mobility impacts of early forms of automated driving—A system dynamic approach," *Transp. Policy*, vol. 72, pp. 171–179, Dec. 2018, doi: 10.1016/j.tranpol.2018.02.013.

[36] Z. Le Hong and N. Zimmerman, "Air quality and greenhouse gas implications of autonomous vehicles in Vancouver, Canada," *Transp. Res. D, Transp. Environ.*, vol. 90, Jan. 2021, Art. no. 102676, doi: 10.1016/j.trd.2020.102676.

[37] J. B. Greenblatt and S. Shaheen, "Automated vehicles, on-demand mobility, and environmental impacts," *Current Sustain. Energy Rep.*, vol. 2, no. 3, pp. 74–81, Sep. 2015, doi: 10.1007/s40518-015-0038-5.

[38] L. M. Martinez and J. M. Viegas, "Assessing the impacts of deploying a shared self-driving urban mobility system: An agent-based model applied to the city of Lisbon, Portugal," *Int. J. Transp. Sci. Technol.*, vol. 6, no. 1, pp. 13–27, Jun. 2017, doi: 10.1016/j.ijtst.2017.05.005.

[39] N. Prakash, G. Cimini, A. G. Stefanopoulou, and M. J. Brusstar, "Assessing fuel economy from automated driving: Influence of preview and velocity constraints," in *Proc. ASME Dyn. Syst. Control Conf.*, vol. 2, Feb. 2017, p. 8, doi: 10.1115/DSCC2016-9780.

[40] Y. Chen, J. Gonder, S. Young, and E. Wood, "Quantifying autonomous vehicles national fuel consumption impacts: A data-rich approach," *Transp. Res. A, Policy Pract.*, vol. 122, pp. 134–145, Apr. 2019, doi: 10.1016/j.tra.2017.10.012.

[41] O. Pribyl, R. Blokpoel, and M. Matowicki, "Addressing EU climate targets: Reducing CO_2 emissions using cooperative and automated vehicles," *Transp. Res. D, Transp. Environ.*, vol. 86, Sep. 2020, Art. no. 102437, doi: 10.1016/j.trd.2020.102437.

[42] K. Mattas *et al.*, "Simulating deployment of connectivity and automation on the Antwerp ring road," *IET Intell. Transp. Syst.*, vol. 12, no. 9, pp. 1036–1044, Nov. 2018, doi: 10.1049/iet-its.2018.5287.

[43] M. Makridis, K. Mattas, C. Mogno, B. Ciuffo, and G. Fontaras, "The impact of automation and connectivity on traffic flow and CO_2 emissions. A detailed microsimulation study," *Atmos. Environ.*, vol. 226, Apr. 2020, Art. no. 117399, doi: 10.1016/j.atmosenv.2020.117399.

[44] O. Kavas-Torris, M. R. Cantas, K. M. Cime, B. A. Guvenc, and L. Guvenc, "The effects of varying penetration rates of L4–L5 autonomous vehicles on fuel efficiency and mobility of traffic networks," SAE Int., Warrendale, PA, USA, Technical Paper, Apr. 2020, doi: 10.4271/2020-01-0137.

[45] V. Zeidler, H. S. Buck, L. Kautzsch, P. Vortisch, and C. M. Weyland, "Simulation of autonomous vehicles based on Wiedemann's car following model in PTV vissim," in *Proc. 98th Annu. Transp. Res. Board Meeting*, 2019, p. 12.

[46] Y. Qin, H. Wang, and B. Ran, "Stability analysis of connected and automated vehicles to reduce fuel consumption and emissions," *J. Transp. Eng. A, Syst.*, vol. 144, no. 11, Nov. 2018, Art. no. 04018068, doi: 10.1061/jtepbs.0000196.

[47] A. Eilbert, L. Jackson, G. Noel, and S. Smith, "A framework for evaluating energy and emissions impacts of connected and automated vehicles through traffic microsimulations," in *Proc. 97th Annu. Transp. Res. Board Meeting*, 2018, p. 18.

[48] B. van Arem, A. P. de Vos, and M. Vanderschuren, "The microscopic traffic simulation model MIXIC 1.3," Dept. Traffic Transp., Transp. Res. Centre, Delft, The Netherlands, Rep. TNO-INRO-VVG 1997-02b, Jan. 1997.

[49] R. Tu, L. Alfaseeh, S. Djavadian, B. Farooq, and M. Hatzopoulou, "Quantifying the impacts of dynamic control in connected and automated vehicles on greenhouse gas emissions and urban NO_2 concentrations," *Transp. Res. D, Transp. Environ.*, vol. 73, pp. 142–151, Aug. 2019, doi: 10.1016/j.trd.2019.06.008.

[50] C. Stogios, D. Kasraian, M. J. Roorda, and M. Hatzopoulou, "Simulating impacts of automated driving behavior and traffic conditions on vehicle emissions," *Transp. Res. D, Transp. Environ.*, vol. 76, pp. 176–192, Nov. 2019, doi: 10.1016/j.trd.2019.09.020.

[51] C. Stogios *et al.*, "Determining the effects of automated vehicle driving behavior on vehicle emissions and performance of an urban corridor," in *Proc. 97th Ann. Transp. Res. Board Meeting*, 2018, p. 17.

[52] H. U. Ahmed, Y. Huang, and P. Lu, "A review of car-following models and modeling tools for human and autonomous-ready driving behaviors in micro-simulation," *Smart Cities*, vol. 4, no. 1, pp. 314–335, Mar. 2021, doi: 10.3390/smartcities4010019.

[53] R. F. Tomás, P. Fernandes, E. MacEdo, J. M. Bandeira, and M. C. Coelho, "Assessing the emission impacts of autonomous vehicles on metropolitan freeways," *Transp. Res. Procedia*, vol. 47, pp. 617–624, 2020, doi: 10.1016/j.trpro.2020.03.139.

[54] *Research on the Impacts of Connected and Autonomous Vehicles (CAVs) on Traffic Flow*, Atkins, Epsom, U.K., 2016.

[55] A. D. Tibljaš, T. Giuffrè, S. Surdonja, and S. Trubia, "Introduction of autonomous vehicles: Roundabouts design and safety performance evaluation," *Sustainability*, vol. 10, no. 4, pp. 1–14, 2018, doi: 10.3390/su10041060.

[56] *SAE International Releases Updated Visual Chart for Its 'Levels of Driving Automation' Standard for Self-Driving Vehicles*, SAE Int., Warrendale, PA, USA, 2018.

[57] M. Michail, M. Konstantinos, C. Biagio, A. R. Maria, T. Tomer, and T. Christian, "Connected and automated vehicles on a freeway scenario. Effect on traffic congestion and network capacity," in *Proc. 7th Transp. Res. Arena*, 2018, pp. 1–10, doi: 10.5281/zenodo.1483132.

[58] J. Auld, V. Sokolov, and T. S. Stephens, "Analysis of the effects of connected–automated vehicle technologies on travel demand," *Transp. Res. Rec.*, vol. 2625, no. 1, pp. 1–8, Jan. 2017, doi: 10.3141/2625-01.

[59] M. Puškár, M. Fabian, J. Kádárová, P. Blišt'an, and M. Kopas, "Autonomous vehicle with internal combustion drive based on the homogeneous charge compression ignition technology," *Int. J. Adv. Robot. Syst.*, vol. 14, no. 5, pp. 1–8, 2017, doi: 10.1177/1729881417736896.

[60] F. Leach, G. Kalghatgi, R. Stone, and P. Miles, "The scope for improving the efficiency and environmental impact of internal combustion engines," *Transp. Eng.*, vol. 1, Jun. 2020, Art. no. 100005, doi: 10.1016/j.treng.2020.100005.

[61] S. G. Farrag, M. Y. El-Hansali, A.-U.-H. Yasar, E. M. Shakshuki, and H. Malik, "A microsimulation-based analysis for driving behaviour modelling on a congested expressway," vol. 11, pp. 5857–5874, May 2020, doi: 10.1007/s12652-020-02098-5.

[62] J. M. Bandeira, P. Fernandes, T. Fontes, S. R. Pereira, A. J. Khattak, and M. C. Coelho, "Exploring multiple eco-routing guidance strategies in a commuting corridor," *Int. J. Sustain. Transp.*, vol. 12, no. 1, pp. 53–65, 2018, doi: 10.1080/15568318.2017.1328545.

[63] Z. Zhai, R. Tu, J. Xu, A. Wang, and M. Hatzopoulou, "Capturing the variability in instantaneous vehicle emissions based on field test data," *Atmosphere*, vol. 11, no. 7, p. 765, Jul. 2020, doi: 10.3390/atmos11070765.

[64] "Methodology for developing modal emission rates for EPA's multi-scale motor vehicle & equipment emission system," North Carolina State Univ., U.S. Environ. Protect. Agency, Ann Arbor, MI, USA, Rep. EPA420-R-02-027, 2002.

[65] P. Fernandes, J. Teixeira, C. Guarnaccia, J. M. Bandeira, E. Macedo, and M. C. Coelho, "The potential of metering roundabouts: Influence in transportation externalities," *Transp. Res. Rec.*, vol. 2672, no. 25, pp. 21–34, 2018, doi: 10.1177/0361198118774667.

[66] D. J. Sheskin, *Handbook of Parametric and Nonparametric Statistical Procedures*. Boca Raton, FL, USA: Chapman Hall/CRC, 2020.

[67] S. D. Horn, "Goodness-of-fit tests for discrete data: A review and an application to a health impairment scale," *Biometrics*, vol. 33, no. 1, p. 237, Mar. 1977, doi: 10.2307/2529319.

[68] E. Macedo, R. Tomás, J. Primo, and M. C. Coelho, "Measuring impacts of 'rat-running' driver behaviour in urban environment using GPS-based traffic data," in *Proc. 23rd EURO Working Group Transp. Meeting*, Paphos, Cyprus, 2020. [Online]. Available: http://hdl.handle.net/10773/29992

[69] D. Dias *et al.*, "Assessing the importance of transportation activity data for urban emission inventories," *Transp. Res. D, Transp. Environ.*, vol. 62, pp. 27–35, Jul. 2018, doi: 10.1016/j.trd.2018.01.027.

[70] S. C. Calvert, W. J. Schakel, and B. van Arem, "Evaluation and modelling of the traffic flow effects of truck platooning," *Transp. Res. C, Emerg. Technol.*, vol. 105, pp. 1–22, Aug. 2019, doi: 10.1016/j.trc.2019.05.019.

[71] R. Fries, Y. Qi, and S. Leight, "How many times should I run the model? Performance measure specific findings from VISSIM models in missouri," in *Proc. Transp. Res. Board Meeting*, 2017, p. 16.

[72] G. Qian and E. Chung, "Evaluating effects of eco-driving at traffic intersections based on traffic micro-simulation," in *Proc. 34th Aust. Transp. Res. Forum*, 2011, p. 11.

[73] Y. Wang and A. Boggio-Marzet, "Evaluation of eco-driving training for fuel efficiency and emissions reduction according to road type," *Sustainability*, vol. 10, no. 11, p. 3891, Oct. 2018, doi: 10.3390/su10113891.

[74] M. S. Alam and A. McNabola, "Network-wide traffic and environmental impacts of acceleration and deceleration among eco-driving vehicles in different road configurations," *Transp. Plan. Technol.*, vol. 41, no. 3, pp. 244–264, Apr. 2018, doi: 10.1080/03081060.2018.1435436.

[75] S. C. Calvert and B. van Arem, "A generic multi-level framework for microscopic traffic simulation with automated vehicles in mixed traffic," *Transp. Res. C, Emerg. Technol.*, vol. 110, pp. 291–311, Jan. 2020, doi: 10.1016/j.trc.2019.11.019.