

Real-Time LNG Buses Emissions Prediction Based on a Temporal Fusion Trans-Formers Model

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ABSTRACT. Emissions from transportation are one of the key factors preventing the achievement of carbon peaking and carbon neutrality by 2050, with particular attention to emissions from buses. Specifically, few research has been conducted on the exhaust emissions characteristics of liquified natural gas (LNG) buses under different driving scenarios. This study proposed a framework for predicting exhaust emissions of LNG buses based on the portable emission measurement system and GPS collaborative perception data. Firstly, the emission distribution characteristics of CO₂, CO, HC, and NO_x from LNG buses in real-world driving were analyzed by visualization methods. Then, the real-time exhaust emissions of LNG buses were predicted based on the temporal fusion transformers model for both urban and suburban sections of Zhenjiang City, and the model validity was verified. The current and past 10 s driving states were used for predicting the emission rate of LNG buses. The results showed that the proposed model outperforms other advanced algorithms in real-time exhaust emissions prediction of LNG buses, with an average R^2 value higher than 0.94 and an average MAPE reduction of 14.19%. The error assessment revealed that the emission values and average emission rates are higher when driving in the urban section compared to the suburban section. Among the influencing factors, traffic conditions have the most significant impacts on the exhaust emissions of LNG buses, followed by road conditions and driving states, with relative feature importance of 48.9, 34.8, and 16.3%, respectively. Additionally, the current and past 10 s driving states also significantly influenced real-time predictions. This study provides an essential theoretical reference for reducing exhaust emissions for city buses.

Keywords: decarbonization, emission prediction, PEMS, GPS, collaborative perception, traffic condition

1. Introduction

To reach the carbon peaking and carbon neutrality goals by 2050, it is necessary to address the crisis of energy security and environmental degradation, improve energy efficiency, reduce greenhouse gas emissions based on current development, and investigate a low-carbon development path for transportation (Pan, 2020). Facing the increasingly critical transportation situation, the National Program for Medium-to-Long-Term Scientific and Technological Development puts forward the strategic objectives of “develop a system and solve three major traffic problems” for transportation science and technology development. Among them, the system refers to the modern comprehensive transportation system; the three major transportation problems include reducing the problem of transportation energy consumption and environmental pollution, solving traffic safety problems, and alleviating traffic congestion problems in large cities. Therefore, it is urgent to accurately understand the carbon emis-

sion levels of city traffic and reduce environmental pollution. The development of public transportation has played a significant role in energy saving and carbon reduction, resulting in an improvement in the traffic pollution situation (Ghaffarpsand et al., 2021). For example, many cities have implemented transit-oriented development, where new energy buses are gradually replacing traditional fuel buses. However, the resulting greenhouse gases such as CO₂ and pollutants such as CO, HC, and NO_x cannot be ignored (Yu et al., 2016; Zhang et al., 2017). Therefore, an in-depth investigation of the exhaust emission characteristics of buses in actual driving is the basis for effective management and control of carbon and pollutant emissions from buses.

Most city buses are equipped with heavy-duty diesel engines, which have high exhaust emission levels (Wang et al., 2018; Shan et al., 2019). More and more buses are switching to new energy power to improve this occurrence (Zhang et al., 2017), so it is vital to re-explore the exhaust emission characteristics of new energy buses. Current city buses can be divided into five categories: 1) diesel-engined buses meeting Euro-IV emission standards (EURO-IV bus); 2) compressed natural gas buses; 3) diesel-engined buses meeting Euro-V emission standards (EURO-V bus); 4) liquefied natural gas bus (LNG bus); and 5) gas-electric hybrid electric bus (GEHE bus). Battery electric buses

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were not considered in this study because they are close to zero exhaust emissions (Wang et al., 2020a). LNG buses have gradually become popular in many cities and are more environmentally friendly than traditional diesel buses.

In addition, blends of diesel and organics are mostly used in aviation engines, and related studies have shown that they have a greater potential as automotive diesel engine fuels due to their good combustion and emission performance. Chen et al. (2017) found a thermal efficiency is 1.4 ~ 12.4% higher than that of diesel fuel and 1 ~ 6.5% higher than that of RP-3 pentanol blends, and that RP-3 and RP-3 pentanol blends significantly reduce soot emissions at high engine loads while increasing CO and HC emissions at low engine loads; Liang et al. (2022) similarly studied diesel fuel, RP-3, and RP-3 pentanol mixtures, quantifying particulate matter (PM) emission concentrations, geometric mean diameter (GMD), and particle size distribution characteristics, and the results showed that the RP-3 pentanol blend significantly reduced PM emissions by 50% less than RP-3 and two orders of magnitude less than diesel; Liang et al. (2023) also compared the combustion and emission characteristics of diesel, RP-3, and synthetic Fischer-Tropsch, and the results showed that, compared to the baseline diesel fuel, combustion of the pentanol-FT mixture (40% PAR) increased CO and HC emissions, and the RP-3 pentanol mixture (40% PAR) increased CO and HC emissions. FT mixture (40% PAR) significantly reduces NO_x by 81% and PM by 75% while thermal efficiency increases by 7.2% compared to the baseline diesel; Raza et al. (2019) added different ratios of dimethyl ether (DME) and n-pentanol (NPENT) to diesel fuel to investigate its combustion and emission characteristics, and the results show that the mixture combustion emits a lower concentration and amount of PM than diesel fuel, and the mixture produces lower NO emissions than diesel fuel at high engine loads, and low combustion emissions are also lower than diesel fuel, and low combustion emissions are lower than diesel fuel. NO emission is also lower than that of diesel, and the mixtures have the best combustion and emission characteristics in low-temperature mode. All of the above studies involved blends such as diesel and pentanol, which suggests that this type of blend has a large potential. However, previous studies have focused on exploring the exhaust emission characteristics of diesel buses (Yu and Li, 2014), passenger cars (Jaikumar et al., 2017), heavy-duty trucks (Abdelmegeed and Rakha, 2017), and GEHE buses (Dreier et al., 2018), with an insufficient exploration of city LNG buses in China (Pan et al., 2019).

The variation of exhaust emissions from city buses is non-linear and depends on complicated external factors. For instance, many studies have considered the effects of factors such as speed, acceleration (Wu et al., 2012), road grade (Wyatt et al., 2014), and traffic flow state (Mahesh and Ramadurai, 2017) on the exhaust emission characteristics of buses. Additionally, city buses exhibit unique operating characteristics in comparison to passenger cars. Due to bus stops and signalized intersections, city buses start, brake, idle, and drive at low speeds much more frequently (Liu et al., 2018), especially in urban sections. For example, Fu et al. (2013) found that NO_x emissions from EURO-IV buses differed when driving in urban and suburban sections. Similarly,

Hao et al. (2010) revealed that exhaust emissions from diesel buses decreased gradually from the city center toward the end of the line. However, the above studies lack a quantitative analysis of exhaust emissions from buses driving in urban and suburban sections.

Achieving accurate estimates of bus exhaust emissions is critical to building a real-time transportation emissions management and control system. Machine learning techniques such as Gradient Boosted Regression Tree (GBRT) (Pan et al., 2019) and Artificial Neural Networks (ANN) (Jaikumar et al., 2017; Antanasijević et al., 2018) have been applied in exhaust emissions prediction. Studies have shown that simultaneously current and past driving states influence bus emissions. However, the above approach of utilizing past driving state data as input in the construction of the model to address the time dependence is not applicable since the effect of past driving states on exhaust emissions is dynamically changing (Hu et al., 2021). As a result, some studies have introduced deep learning architectures to compensate for this deficiency. Long Short-Term Memory (LSTM), a deep learning model for analyzing the temporal correlation of data, possesses great potential for bus emission prediction (Sun et al., 2021). Yu et al. (2021) pointed out that few studies have used deep learning algorithms to develop prediction models for diesel bus NO_x emissions and demonstrated that the LSTM model shows good learning and prediction capabilities for instantaneous changes in NO_x emissions. According to existing studies, Gated Recurrent Unit (GRU) networks can handle the time dependence of the exhaust emission data (Fanta et al., 2020). More importantly, the prediction accuracy of the GRU network is comparable to that of LSTM, and the more simplified structure and fewer parameters of GRU can effectively reduce the training time (Wang et al., 2020b). However, the application of Deep Neural Networks (DNN)-based architectures for bus exhaust emission prediction has not been found. DNN-based architecture is a branch of deep learning. It has been shown to address time-dependent robust performance improvements (Lim et al., 2021), and this study proposes to investigate its feasibility for carbon and other pollutant emission prediction from city LNG buses.

The driving condition parameters, including vehicle speed, acceleration, heading angle, altitude, etc., have been proved to have significant effects on exhaust emission (Wu et al., 2012). Since these parameters are time series, the TFT model was developed to predict the exhaust emission of LNG buses. The TFT model can fully understand and utilize the relationship between multiple time series features (Wen et al., 2017; Fan et al., 2019), and it can accurately capture the complex dependency relationship between the exhaust emission and driving conditions. In addition, the data collection interval is 2 s, the data scale is large. The TFT model has parallel computing capability (Lim et al., 2021), which helps to deal with the training and prediction speed and efficiency. Currently, the TFT model can be applied in industries such as transportation, electricity, retail, and stock (Lim et al., 2021), but no study has applied it for predicting the exhaust emissions of LNG buses.

The above research gaps can be summarized as follows. First, some studies (Liu et al., 2018; Wang et al., 2020) have

examined the exhaust emission characteristics of traditional fuel buses. Still, there are insufficient studies on new energy buses, especially LNG buses. Furthermore, there is a lack of quantitative analysis of exhaust emissions from LNG buses when driving in urban and suburban sections. Second, most studies only consider the effect of the current driving state on bus exhaust emissions (Liu et al., 2013; Shan et al., 2018). In reality, bus emissions are also influenced dynamically by past driving states (Qi et al., 2004). Additionally, most relevant studies (Pan et al., 2019) currently employ machine learning algorithms widely used to predict bus exhaust emissions. In contrast, novel deep learning algorithms with interpretable attention-based mechanisms are insufficiently employed in this field.

2. Literature Review

2.1. Factors Affecting Bus Exhaust Emissions

Many studies are currently evaluating the exhaust emissions performance of city buses to help scientists, city policy-makers, and bus companies achieve economic and decarbonized public transportation. According to existing research, the main factors affecting bus exhaust emissions can be divided into two categories: one is the factors related to the bus, such as driving speed and acceleration (Pan et al., 2020); the other is the road traffic conditions factors, such as the degree of congestion, road slope (Rosero et al., 2021).

Domestic and foreign studies have focused on exploring the effects of factors such as speed and acceleration on exhaust emissions characteristics. Buses differ from other vehicle types in that their exhaust emissions performance can be impacted by frequent stop-and-go driving behaviors in city environments. It may also contribute to traffic congestion and affect other vehicles (Lv and Zhang, 2012; Özener and Özkan, 2020). For the speed and acceleration factors, Choudhary et al. (2016) found that the sharp changes in acceleration and deceleration were the leading cause of carbon and pollutant emissions from buses. Additionally, Qi et al. (2004) assessed the effect of speed and acceleration persistence on vehicle emission characteristics. The results show that exhaust emissions are affected by speed and acceleration at the current moment and in the past few seconds. Therefore, this study focused on analyzing and quantifying the carbon and pollutant emissions of buses under different driving conditions and considered the effects of past driving conditions during prediction.

Road traffic conditions can significantly affect the exhaust emission characteristics of buses. In this regard, domestic and foreign studies have concentrated on factors such as road slope and traffic congestion status. In their analysis of the impact of road slope on vehicle CO₂ emission rates, Wyatt et al. (2014) demonstrated how ignoring road slopes when driving could compromise the accuracy of CO₂ emission rate predictions. In addition, García et al. (2014) thoroughly investigated the effect of traffic congestion status on vehicle emissions characteristics. The results demonstrated that vehicle exhaust emissions increased dramatically in congested traffic compared to free-flow conditions. Similar studies by Manesh et al. (2017) and Wang

et al. (2018) on bus emissions, during peak and off-peak hours discovered that peak hours had significantly higher total emissions of all polluting gases. Based on the above analysis, this study considers the effects of road and traffic conditions on the exhaust emissions of LNG buses. Moreover, research (Hu et al., 2021) has shown that bus stops and intersections are where almost half of the bus emissions originate. However, they are not evenly dispersed across the bus line, and often urban sections are denser, leading to more complex traffic conditions. Therefore, it is necessary to explore further the differences in exhaust emissions of buses driving in urban and suburban sections, which is one of the studies in this paper. Several of the above studies adopted the Portable Emission Measurement System (PEMS) to obtain real-time emission data, which has become a crucial tool for examining the exhaust emission characteristics of vehicles in real-world driving (Rosero et al., 2020) and is the data acquisition method chosen for this study.

2.2. Bus Exhaust Emissions Prediction

Achieving real-time and accurate estimation of bus exhaust emissions is also one of the current research priorities. Machine learning and deep learning algorithms have been frequently applied to vehicle emissions prediction (Pan et al., 2019). Many studies (Qi et al., 2004) have shown a strong time dependence between exhaust emissions and vehicle operation, which may be more pronounced for buses, as they frequently accelerate and decelerate at bus stops and intersections. Jaikumar et al. (2017) applied the ANN model to estimate the real-time bus emissions and demonstrated its feasibility. To solve the nonlinear problem more effectively, Pan et al. (2019) utilized the GBRT model for real-time bus emission prediction considering the time dependence, and the results showed the good predictive performance of the model. The above studies address the time dependence problem utilizing historical driving state data. However, using the past one or ten seconds of data as input in building the model is too simplistic since not all historical driving states significantly affect current exhaust emissions. To remedy this deficiency, Sun et al. (2021) introduced the LSTM model, which can adaptively decide whether to forget the past driving state by the forgetting gate at each time step. The results indicate that the LSTM model significantly improves accuracy compared with the traditional model. Therefore, this paper exploits LSTM to deal with the effect of past inputs on bus exhaust emission prediction. The TFT model uses an LSTM Encoder-Decoder to locally process the temporal dependence of the feature inputs and reasonably assign the time-varying contribution weights of the feature inputs to the exhaust emissions based on the multi-head attention mechanism. This is the significant cause for choosing the TFT model for bus exhaust emission prediction in this study. In addition, the TFT model takes bus travel time as the known input, which may significantly impact exhaust emission prediction, a detail commonly ignored by previous prediction algorithms. More importantly, the TFT model exhibits good interpretability by dynamically filtering the significant variables for exhaust emission prediction based on the variable selection networks at each time step.

2.3. The Contributions of This Paper

The main objective of this study is to analyze the distribution characteristics of the exhaust emissions from LNG buses in actual driving and to accurately predict the real-time emission rate using deep learning algorithms. The main contributions of this study are as follows: 1) the exhaust emissions distribution characteristics of CO₂, CO, HC, and NO_x of LNG buses were analyzed in terms of traffic conditions, driving state, and road conditions based on PEMS and GPS collaborative perception data; 2) the TFT model was constructed to predict the emission rates of the four exhaust gases of LNG buses, and the prediction results were compared with other advanced algorithms using three evaluation indicators, RMSE, MAE, and MAPE; 3) the performance of the TFT model was further validated based on MAPE after comparing the emission prediction results of urban and suburban sections; and 4) the feature importance of exhaust emissions were quantified based on the variable selection network of the TFT model.

The remainder of this paper is structured as follows. Section 3 presents the methodology of this study. Section 4 introduces the data sources and analyzes LNG buses exhaust emission distribution characteristics. Section 5 predicts the real-time exhaust emissions of LNG buses and validates the model's performance by comparing the prediction results with other advanced algorithms. Finally, the conclusions of this study and recommendations for further research are summarized in Section 6.

3. Methodologies

3.1. Framework

Significant differences exist in CO₂, CO, HC, and NO_x emissions between LNG and traditional fuel buses (Pan et al., 2019). The following methods were considered in this study to understand further the distribution characteristics of the four exhaust emissions of LNG buses and to predict the real-time emissions accurately.

Analyze LNG buses exhaust emission distribution characteristics under different driving conditions. This study divides the driving conditions into three categories: traffic conditions, which refer to the travel time of the LNG bus, i.e., peak or off-peak hours; driving state, which is expressed by speed and acceleration; and road conditions, including road slope and turning angle (the leg course of the vehicle).

Predicting real-time exhaust emissions of LNG buses in actual driving based on the TFT model. Considering that not all historical driving states significantly affect the exhaust emissions at the current moment, the TFT model using LSTM Encoder-Decoder can locally handle the time-dependent relationship of feature inputs and reasonably assign the time-varying contribution weights of feature inputs to exhaust emissions based on the multi-head attention mechanism.

Validate the performance of the TFT model for the four exhaust emission predictions of LNG buses. This study compares

six typical gradient enhancement algorithms for urban and suburban sections with the TFT model. It uses RMSE, MAE, and MAPE as evaluation indicators to assess the prediction performance of the above methods.

The feature importance analysis is developed in the end. Identifying the impact of the above factors on exhaust emissions can provide an essential reference for carbon reduction and pollution mitigation measures.

3.2. Predicting Exhaust Emissions of LNG Buses Based on the TFT Model

This study aims to explore the correspondence between LNG bus emissions and explanatory variables and achieve accurate emission prediction based on the TFT model. Previous studies show vehicle emissions are influenced by current and past driving states. There is a potential role for other known information (e.g., whether it is in peak hours). Therefore, in this study, the current and past 10 s driving states (denoted as X_{t-it} , y_{t-it} , $i = 9$) and known information (denoted as F_{t+1}) were used as model inputs to predict the emission rate of LNG buses. The emission prediction model is expressed as equation (1):

$$\hat{y}_{t+1}^m = f(l, X_{t-it}, y_{t-it}, F_{t+1}) \quad (1)$$

where l is a static covariate (does not vary over time), and in this study, l refers to fuel type; t is the time; m is the type of LNG bus emissions, including CO₂, CO, HC, and NO_x; \hat{y}_{t+1}^m denotes the emission rates of the four exhaust gases from the LNG bus at time step $t + 1$; i represents the maximum past time step, and $i = 9$ s in this study; X_{t-it} denotes the driving state at the current moment and in the past i s, and indicates the emission rate at the corresponding time; F_{t+1} represents the known information at time step $t + 1$.

The exhaust emission prediction model of equation (1) shows the nonlinear relationship between current and past driving states, and known information and emission rate. Although the prior information on how the multi-source feature inputs interact with the emission rates is unknown, the TFT model is constructed with flexibility to solve the time-dependent problem and demonstrate good interpretability. Figure 1 shows the framework of real-time exhaust emission prediction for LNG buses based on the TFT model. The TFT model is a DNN architecture based on the attention mechanism (Lim et al., 2021). The model first uses the variable selection networks to dynamically filter significant variables for exhaust emission prediction at each time step, providing greater flexibility than previous algorithms that assigned fixed weights to all feature inputs. Then LSTM Encoder-Decoder is employed to solve the discrepancy problem of multi-source feature dimensionality and locally handle the temporal relationship of feature inputs. In addition, a multi-head attention mechanism is applied to avoid the model over-focusing on partial features, and the time-varying contribution weights of feature inputs to exhaust emissions are reasonably assigned. Therefore, the TFT model is the appropriate selection to accurately predict LNG buses' exhaust emissions.

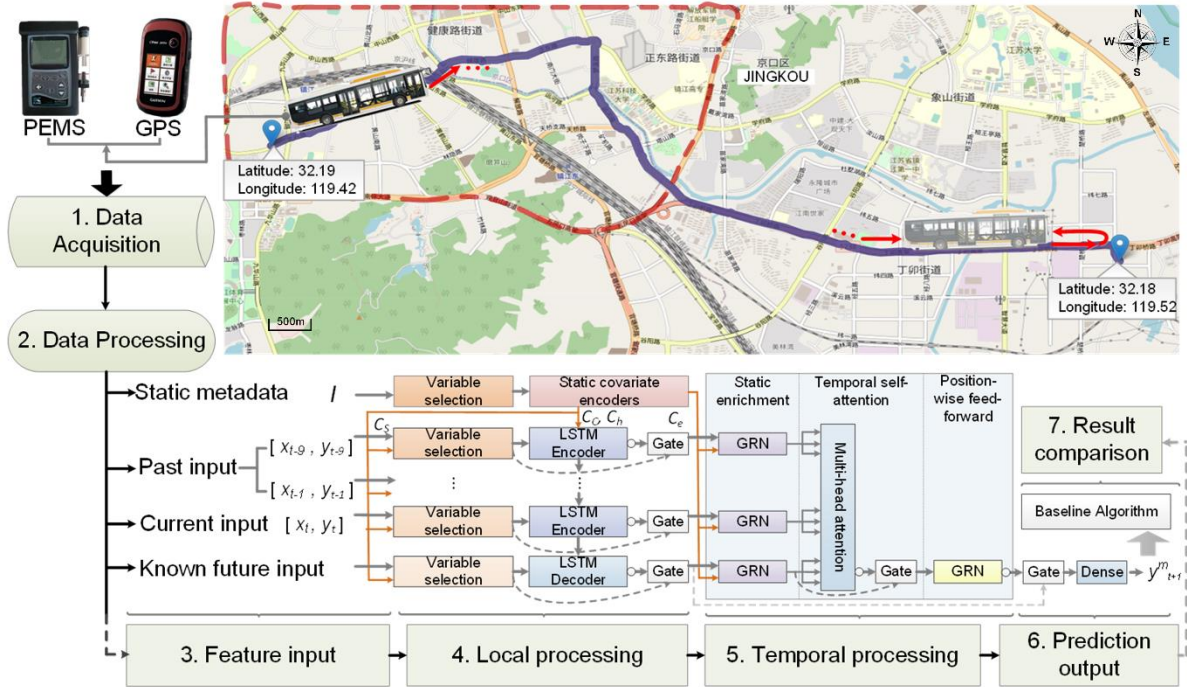


Figure 1. Real-time exhaust emission prediction framework for LNG buses based on the TFT model.

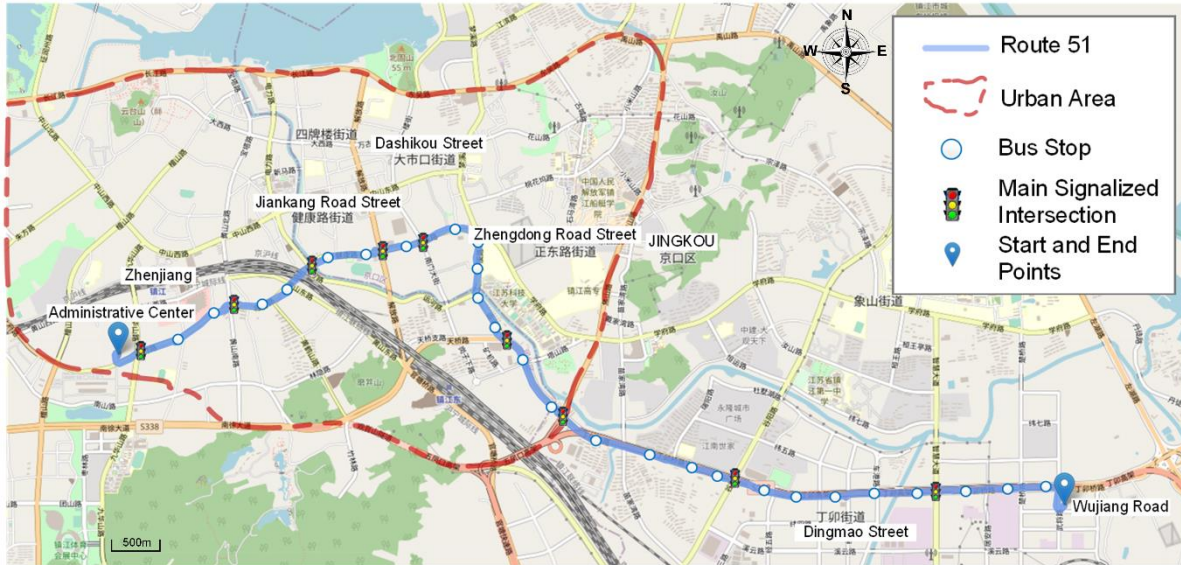


Figure 2. Location of bus line 51.

4. Analysis of Exhaust Emissions Distribution Characteristics of LNG Buses

4.1. Data

The data collection experiment for LNG buses was conducted on April 12 (Tuesday), 2016, in Zhenjiang, China. Figure 2 shows the geographical location of the bus line. The total length of the bus line is about 11.5 km, of which the length of

the urban section accounts for approximately half. There are plenty of hills within Zhenjiang, meaning road conditions must be considered. The measured buses were operated with the air conditioning system off, and the dataset was gathered in favorable weather circumstances.

Additionally, collecting data during peak and off-peak hours excludes effects arising from traffic conditions. The experiment adopted PEMS to measure LNG buses' CO₂, CO, HC, and NO_x emissions under actual traffic conditions. Moreover, the handheld

GPS 16-HVS device is employed to record the real-time location, road slope, and speed information of LNG buses.

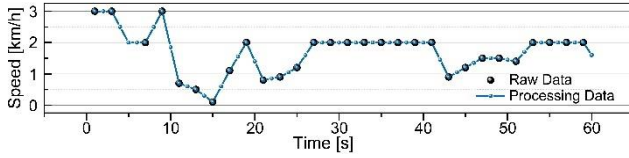


Figure 3. Example of linear interpolation.

The GPS device obtains position data every 2 seconds, and the PEMS device records exhaust emission data every 2 to 3 seconds. Therefore, data cleaning and fusion processing methods are needed to improve data quality. In this paper, a linear interpolation method is used to obtain second-by-second driving data and emission data, and the two parts are fused into one dataset. Figure 3 shows an example of linear interpolation. In addition, since the TFT model can handle multi-source feature inputs and integrate the effects of static and known inputs on LNG bus exhaust emission prediction, this study tries to supplement as much as possible the relevant data available, including the travel time, fuel type, and acceleration of LNG buses. The final parameter interpretation is shown in Table 1.

The data collected by the experimental equipment has the problem of missing data, which will lead to the incompleteness of the time series and ultimately affect the performance of the model prediction. As shown in Figure 3, this study uses linear interpolation to supplement the missing data, Rippa (1992) proves that linear interpolation is suitable for supplementing the missing data of time series, and Pan et al. (2019) also uses linear interpolation to supplement the actual data, and it is feasible to use linear interpolation to supplement the missing data of the time series, which ensures the characteristics of the time series and the accuracy of the model prediction.

4.2. Exhaust Emissions Distribution Characteristics

The wide range of LNG buses exhaust emission rates may be influenced by a variety of factors in actual traffic. This study examines the traffic, driving, and road conditions to investigate

carbon and pollutant emission distribution characteristics of LNG buses under various driving scenarios.

4.2.1. Traffic Condition

Off-peak and peak hours typically exhibit considerable changes in traffic conditions. Figure 4 shows the distribution of exhaust emissions from LNG buses when driving during off-peak and peak hours. The emission rate per second (Emission Rate 1) and emission rate per meter (Emission Rate 2) are adopted as emission indicators. For LNG buses driving during off-peak hours, the CO₂ emission rate 1 is 8.27%, and emission rate 2 is 1.57%; the CO emission rate 1 is 0.09%, and emission rate 2 is 0.02%; the HC emission rate 1 is 0.17%, and emission rate 2 is 0.003%; and the NO_x emission rate 1 is 0.16%, and emission rate 2 is 0.03%. For LNG buses driving during peak hours, the CO₂ emission rate 1 is 8.47%, an increase of 2.42% relative to off-peak hours, and the emission rate 2 is 2.24%, a relative increase of 42.68%; the CO emission rate 1 is 0.11%, a relative increase of 25.09%, and the emission rate 2 is 0.03%, a relative increase of 76.69%; the HC emission rate 1 is 0.16%, a relative decrease of 8.08%, and the emission rate 2 is 0.004%, a relative increase of 27.88%. The NO_x emission rate 1 is 0.15%, a relative decrease of 9.72%, and the emission rate 2 is 0.04%, a relative increase of 26.71%. The emission rates per meter for all four exhaust gases increased dramatically for LNG buses driving during peak hours relative to off-peak hours. The emission rates per second (except for CO emission) increased insignificantly or even decreased marginally. Analysis of the driving environment shows that the road traffic flow is higher during peak hours. LNG buses may therefore produce more complex driving behaviors. The average speed is slower, and delays are increased, so the emission rate per meter of the four exhaust gases is significantly higher. In contrast, the emission rate per second may be reduced. However, prolonged low-speed driving and stop-and-go conditions can lead to insufficient fuel combustion, which is one of the reasons why the CO emission rate per second increases significantly. It means that driving behavior on LNG buses is influenced by external traffic conditions, which substantially impact exhaust emissions, especially carbon oxides.

Table 1. Description of Exhaust Emission Variables

NO.	Classification	Parameters	Unit	Description
1	Static	fuel_type	-	Fuel type of the LNG bus
		altitude	m	The altitude of the road
2	Observed	leg speed	km/h	Speed of the LNG bus
		acceleration	m/s ²	Acceleration of the LNG bus
		leg course	°	The heading angle of the LNG bus
3	Known	is_peak	-	Whether it is during the peak hours
		time_on_day	-	Travel time of the LNG bus
4	Target	CO ₂	%	CO ₂ emission rate
		CO	%	CO emission rate
		HC	%	HC emission rate
		NO _x	%	NO _x emission rate

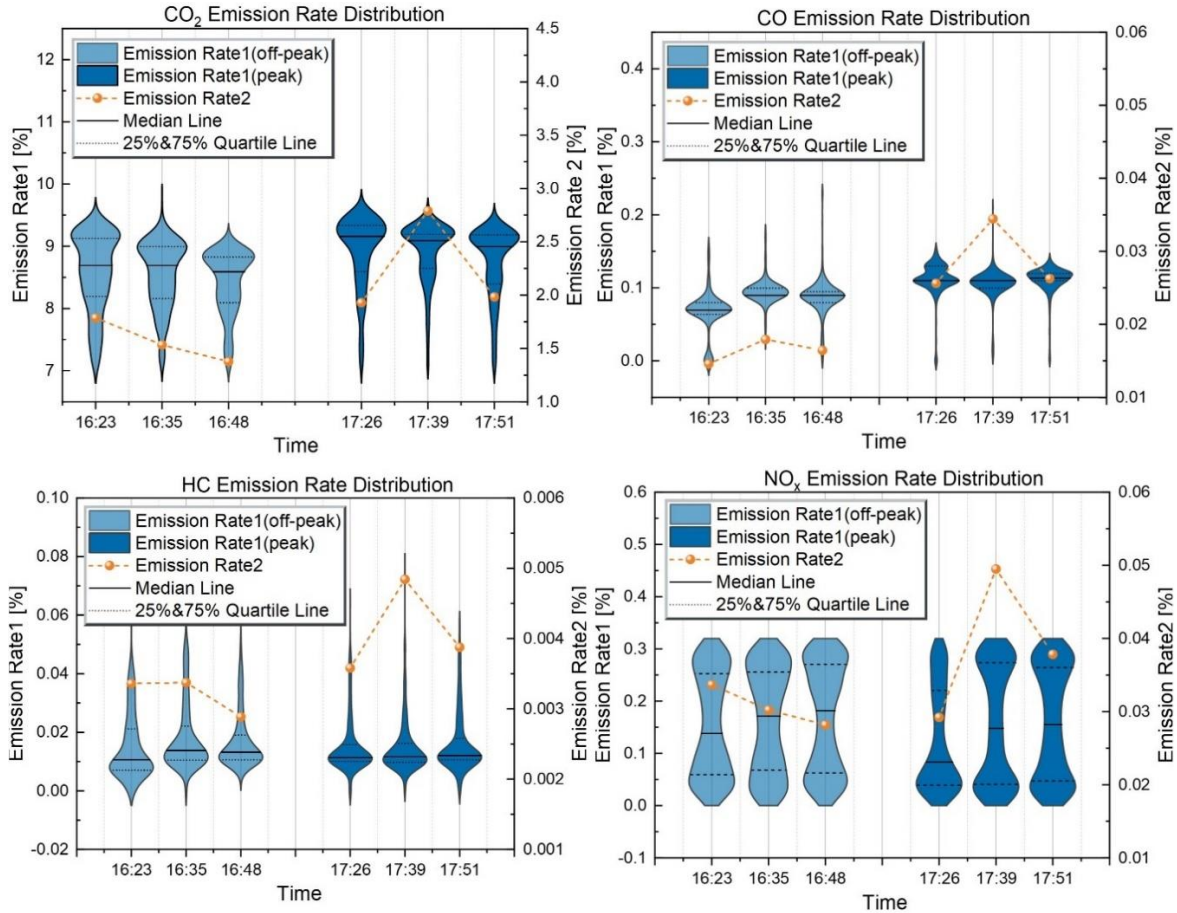


Figure 4. Exhaust emission distribution of LNG buses driving during off-peak and peak hours.

4.2.2. Driving Status

Speed and acceleration are usually employed to describe the driving state of a vehicle. Figure 5 displays the heat maps of speed, acceleration, and the four exhaust emission rates. Based on the distribution of speed and acceleration, the driving states of LNG buses are divided into seven main categories: 1) LsA (Low speed & Acceleration); 2) LsD (Low speed & Deceleration); 3) HaA (High speed & Acceleration); 4) HsD (High speed & Deceleration); 5) LCs (Low & Constant speed); 6) HCs (High & Constant speed); 7) Ts (Temporary stop).

The exhaust emission rates for different driving states are summarized in Table 2. The results show that the braking of LNG buses at low speeds, as opposed to acceleration, leads to an increase in exhaust emissions, especially the NO_x emission, by 30.46%; the effect of acceleration and deceleration at high speeds on the four exhaust emissions is not apparent; the CO₂, CO, and NO_x emissions of LNG buses are higher under the HCs driving state than under the LCs driving state, with the NO_x emission exhibiting the most notable performance, which indicates that increased speed leads to an increase in CO₂, CO, and NO_x emissions, and the NO_x emission are more sensitive to changes

in driving state; there is a decreasing trend in HC emissions as the speed increases; the Ts driving state includes temporary stops at bus stops and queues at intersections, which last longer during peak hours and result in additional exhaust emissions from LNG buses. In addition, LNG buses emit the highest HC emission rate under the Ts driving state. Therefore, by analyzing the above driving states, it can be concluded that LNG buses can effectively reduce carbon and pollutant emissions by driving at moderate speeds and making slight acceleration and deceleration adjustments during actual driving.

4.2.3. Road Condition

This study analyzed the relationship between the real-time leg course (i.e., heading angle) variation and the four exhaust emission rates of the LNG bus. In Figure 6(a), CO₂, CO, and HC emission rates are most significant at 80 ~ 100° change in leg course when the LNG bus typically turns at intersections; when driving on a flat road (with a value of 0° change in leg course), LNG buses emit the highest NO_x emission but significantly decrease when steering. Road curvature directly impact

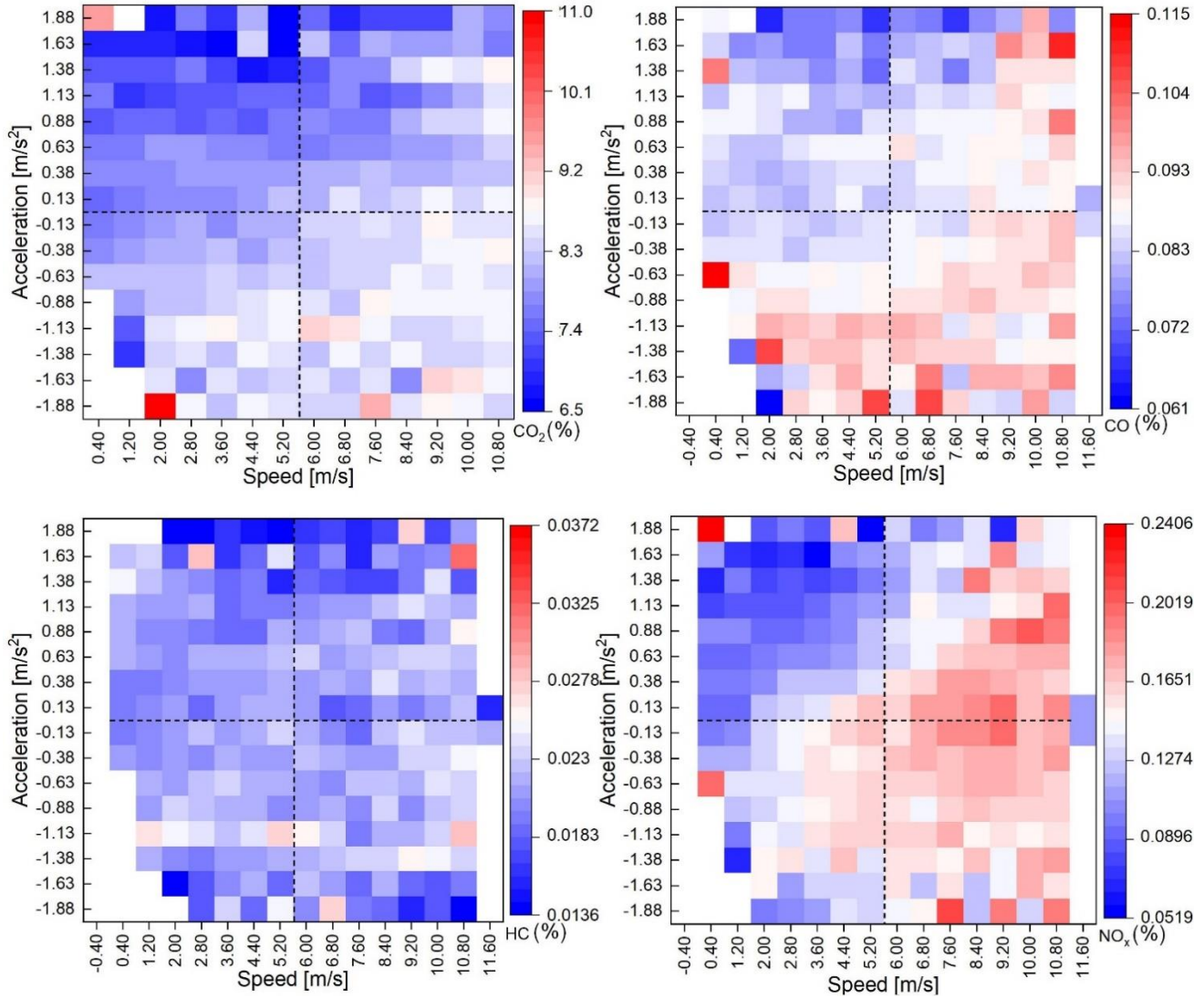


Figure 5. Heat maps of speed, acceleration, and exhaust emission rates of LNG buses: (a) CO₂; (b) CO; (c) HC; (d) NO_x.

Table 2. Average Emission Rates of Exhaust Gases under Different Driving States

		LsA	LsD	HsA	HsD	LCs	HCs	Ts
Average	CO ₂	8.06	8.11	8.21	8.35	8.23	8.35	7.78
Emission	CO	0.09	0.09	0.10	0.09	0.09	0.10	0.08
Rate (%)	HC	0.02	0.02	0.02	0.02	0.02	0.02	0.03
	NO _x	0.10	0.15	0.23	0.22	0.09	0.23	0.07

the change in the leg course of LNG buses, and it indirectly affects exhaust emissions. Another factor related to road conditions is the road slope. In Figure 6(b), the real-time altitude variation (Δ Altitude) indicates the uphill and downhill driving states of the LNG bus, which Δ Altitude $\in [-5,0)$ expresses downhill driving, Δ Altitude = 0 denotes that the bus is driving on a gentle road, and Δ Altitude $\in (0,5]$ represents uphill driv-

ing. It can be observed that there are differences in the effects of different uphill and downhill driving states of LNG buses on the four exhaust emission rates. LNG buses emit less CO₂ and CO when driving downhill, reducing emissions by 1.72% and 2.22%, respectively; HC and NO_x emissions are lower when driving uphill, reducing emissions by 7.06 and 6.80%, respectively.

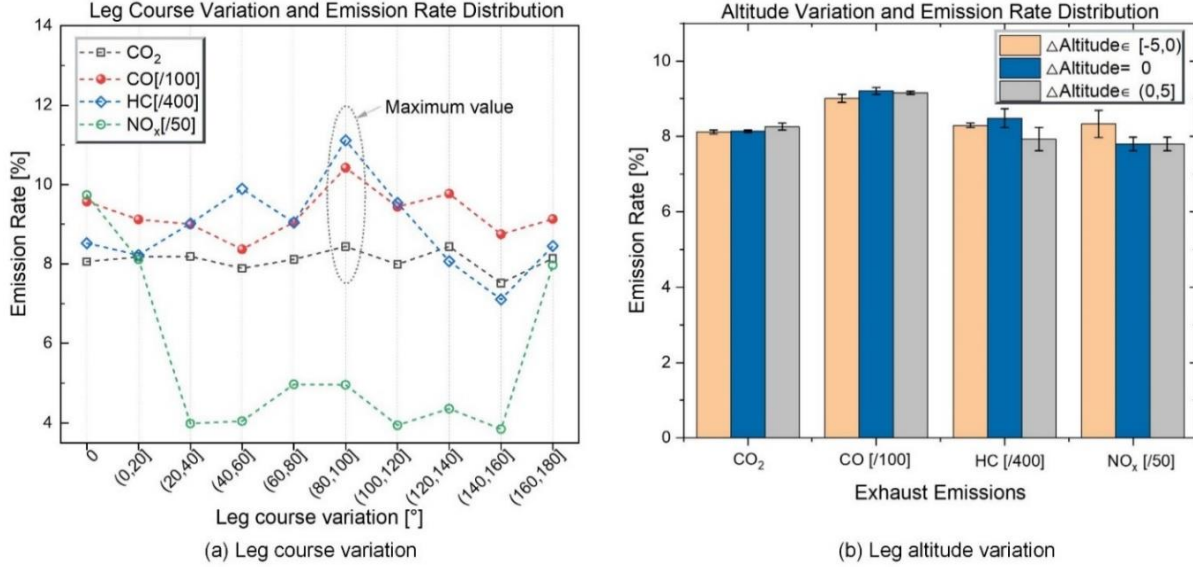


Figure 6. Emission rate distribution of the four exhaust gases under different leg courses and leg altitude variations.

Table 3. Results of the Optimal Parameters of the TFT Model

Parameters	CO ₂	CO	HC	NO _x
learning_rate	0.01	0.01	0.01	0.001
num_heads	4	4	4	4
dropout_rate	0.3	0.2	0.4	0.3
hidden_layer_size	320	320	240	320

5. Results and Discussion

5.1. Model Development

This subsection provides further detailed information about the construction and training of the TFT model. First, 80% of the data is assigned as the training set, and the remaining 20% as the test set. The multi-source features are then fed into the respective variable selection network for training. The training set is subsampled (at a sampling rate of 10%) for network calibration. Six different history lengths of data, 6, 8, 10, 12, 14, and 16 s, were selected to compare the quantile loss function, the results showed that the model results were best when the length was 10 s, and the length of history time was determined to be 10 s. The training process was iterated 500 times to ensure reliable prediction results. In addition, to construct the best TFT model, this optimized study parameters that usually have a significant impact on model performance, including learning_rate (i.e., the initial learning rate of ADAM optimizer, taking values in the range of [0.001, 0.1]), num_heads (i.e., number of heads for interpretable multi-head attention, taking values in the range of [1, 4]), dropout_rate (i.e., dropout discard rate, taking values in the range of [0.1, 0.9]), and hidden_layer_size (i.e., internal state size of TFT, taking values in the range of [10, 320]). Hyperparameter optimization was performed by random search, using 240 iterations for volatility and 60 iterations for other parameters, finally outputting the optimal model parameters. The final TFT model was trained based on the data from four exhaust emis-

sions, and the parameter combinations for each training result are summarized in Table 3.

5.2. Model Validation

Machine learning algorithms have been applied to the field of vehicle emissions prediction. Among them, the gradient boosting algorithm utilizes multiple estimators to create a more stable and robust algorithm with high accuracy. In this study, several typical gradient boosting algorithms are employed to compare the prediction performance of the TFT model, including eXtreme Gradient Boosting (XGBoost), Light Gradient Boosting Machine (LightGBM), CatBoost, Adaptive Boosting (AdaBoost), and gradient boosted regression tree (GBRT). This paper utilizes Root Mean Square Error (RMSE), Mean Absolute Error (MAE), and Mean Absolute Percentage Error (MAPE) to evaluate the prediction results of LNG bus exhaust emissions. The RMSE is defined using expression in Equation (2), the MAE is defined using expression in Equation (3), and the MAPE is defined using expression in Equation (4):

$$RMSE = \sqrt{\frac{1}{m} \sum_{j=1}^m (\hat{y}_j - y_j)^2} \quad (2)$$

$$MAE = \frac{1}{m} \sum_{j=1}^m |y_j - \hat{y}_j| \quad (3)$$

$$MAPE = \frac{100\%}{m} \sum_{j=1}^m \left| \frac{\hat{y}_j - y_j}{y_j} \right| \quad (4)$$

where $\{\hat{y}_1, \hat{y}_2, \dots, \hat{y}_m\}$ is the predicted value and $\{y_1, y_2, \dots, y_m\}$ is the observed value. Accurate prediction results correspond to smaller RMSE, MAE, and MAPE values.

Table 4. Prediction Performance Comparison between the TFT Model (in Bold) and Other Advanced Algorithms

Model	RMSE (%)				MAE (%)				MAPE (%)			
	CO ₂	CO	HC	NO _x	CO ₂	CO	HC	NO _x	CO ₂	CO	HC	NO _x
Adaboost	1.18	0.29	1.02	6.71	0.71	0.14	0.81	5.59	8.95	15.40	28.37	30.58
GBRT	1.11	0.29	0.85	5.45	0.66	0.20	0.55	3.67	8.75	16.12	27.10	31.31
XGBoost	1.34	0.33	1.02	6.66	0.81	0.15	0.73	5.21	9.32	15.33	30.19	36.87
LightGBM	1.40	0.35	1.13	6.78	0.84	0.19	0.86	5.38	8.21	14.62	33.30	30.79
Catboost	1.10	0.27	0.84	5.30	0.61	0.13	0.60	3.93	8.20	11.78	32.00	31.24
MLP	2.99	0.59	2.01	12.28	2.47	0.44	1.56	10.06	12.30	5.45	19.45	14.35
TFT	0.36	0.05	0.27	1.41	0.20	0.03	0.17	0.90	2.42	4.23	10.86	6.69

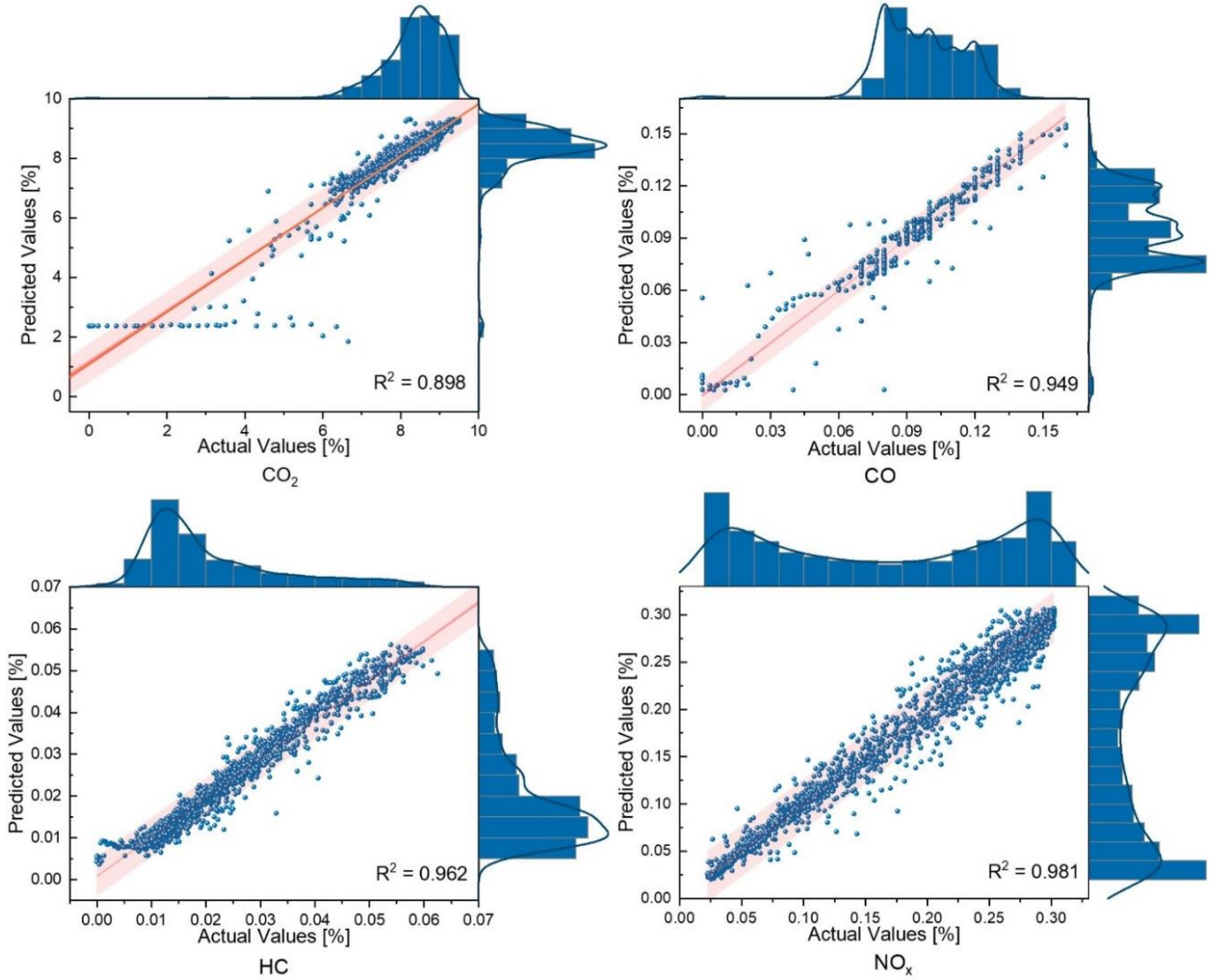


Figure 7. Prediction results and statistical distribution of LNG bus exhaust emissions based on TFT modeling.

5.3. Result Analysis

5.3.1. Prediction Results Validation

Figure 7 shows the predicted CO₂, CO, HC, and NO_x emission rates with R^2 values of 0.898, 0.949, 0.962, and 0.981, respectively. It can be seen that the R^2 values are all greater than 0.89, which indicates that more than 89% of the variability characteristics of the four exhaust emissions of LNG buses can be

explained utilizing the variables in Table 1. Table 4 summarizes the model validation results for LNG buses. As an innovative deep learning algorithm, the TFT model performs optimally for the prediction of four exhaust emission substances for LNG buses, achieving significant MAPE reductions of 5.78, 7.55, 19.33, and 24.10%, respectively. In addition, the Cat-Boost model presents less error than other comparison algorithms. The main ad-

vantage is that it identifies the category variables in the feature inputs, namely is_peak and time_on_day in Table 1, which the TFT model inputs into the LSTM Decoder as available features. In addition, it can be observed that the MAPE value for the HC emission is 10.86%, which is lower than the prediction error of other advanced algorithms. Still, the results of the cross-sectional comparison are slightly worse. Combined with the observed data and the analysis in Section 4.2, the possible reason is that HC emissions from LNG buses are insensitive to changes in driving states, making it challenging to capture the actual changing characteristics of HC emissions when using past driving states for prediction. We plotted the loss function of the training and test datasets in Figure 8, and as the number of iterations increases, the loss of both the training and test sets decreases, and all the curves show a decreasing trend, with no other changes, so there is no problem of over-training.

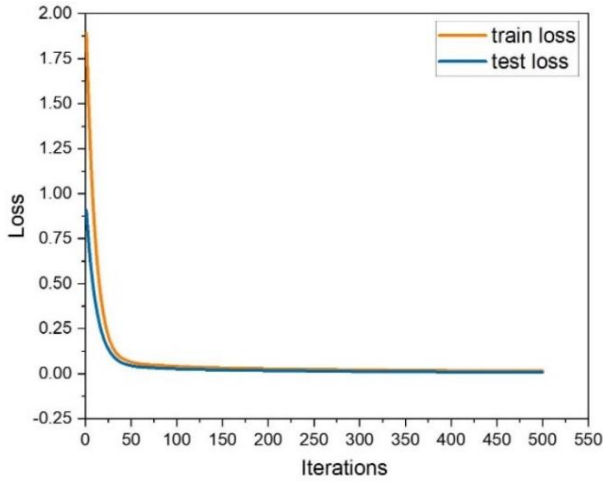


Figure 8. Loss plots for training and prediction datasets.

We conducted a robustness study of the TFT model. We calculated quantile loss functions for four gases, including the 10% loss function, 50% loss function, and 90% loss function as Table 5. The quantile loss function makes the model more robust against outliers. Since it treats the errors under different quartiles separately, the model is better able to maintain stability in the presence of outliers or anomalies. In addition, the quantile regression model shown in Figure 9 provides information about different quartiles that can be used to explain the prediction results in different situations. With the quantile loss function and quantile prediction, we found that the TFT model is robust to the four gas predictions and has better stability.

5.3.2. Prediction Results Comparison and Error Analysis

In addition to comparing the selected models at the macro level, this subsection further validates the prediction performance of the TFT model on different road sections. Figure 10 shows the geographic locations of the two test sections, which are located in urban and suburban areas, both around 4 km in length. The urban section (section 1) has a maximum altitude

change of 88 m. In contrast, the suburban section (section 2) is relatively gentle, with a maximum altitude change of 16 m. Additionally, it can be seen that the course change of LNG buses is more complicated when driving on section 1. The statistical information for the two test sections is summarized in Table 6. The number of bus stops is the same for both sections, but the bus stop spacing in section 1 is relatively shortened by about 5%; the number of intersections in section 1 has increased by 8, and the intersection spacing has been reduced by approximately 43%; the average speed of LNG buses in urban areas is significantly lower than in suburban areas, mainly related to the more complex traffic conditions in urban sections.

Table 5. TFT Model Results for Exhaust Emission Quantile Loss Functions

	P10_Loss	P50_Loss	P90_Loss
CO ₂	0.07	0.13	0.18
CO	0.19	0.28	0.14
HC	0.24	0.69	0.47
NO _x	0.38	0.59	0.77

Table 6. Statistical Information for the Two Test Sections

Name	Road section 1	Road section 2
Number of bus stops	9	9
Number of intersections	20	12
Average bus stop spacing (m)	400	420
Average intersection spacing (m)	200	350
Average speed (km/h)	15.98	20.09

Figure 11 compares the actual emission distributions for the test sections with the predicted results from the TFT model and other advanced algorithms. The CatBoost model is chosen here for comparison with the TFT model since it performs best in the comparison algorithms in the analysis discussed above. Overall, the predicted results of the TFT model for the four exhaust emissions on the two test sections were very similar to the actual distribution. In contrast, the predicted results of the CatBoost differed more obviously from the actual distribution. In addition, LNG buses have a more excellent range of emission values and emission rates for the four exhaust gases when driving in the urban section compared to the suburban section, with a relative increase of 53.9% in CO emission rates in particular. It is related to the fact that the urban section has more stops, queues, turns, and uphill and downhill driving, resulting in stop-and-go driving states for LNG buses, especially during peak hours.

Therefore, from the macro level of promoting low-carbon travel in city buses, it is worth paying more attention to the exhaust emissions of new energy buses in urban sections. One approach worth considering is to provide bus-only lanes at specific intersections to reduce delays from bus interactions with other vehicles, which is more applicable in urban sections with a high density of bus stops and intersections. Another feasible measure is to design green wave traffic based on the intelligent platform to enable intelligent traffic signals and multi-point linkage

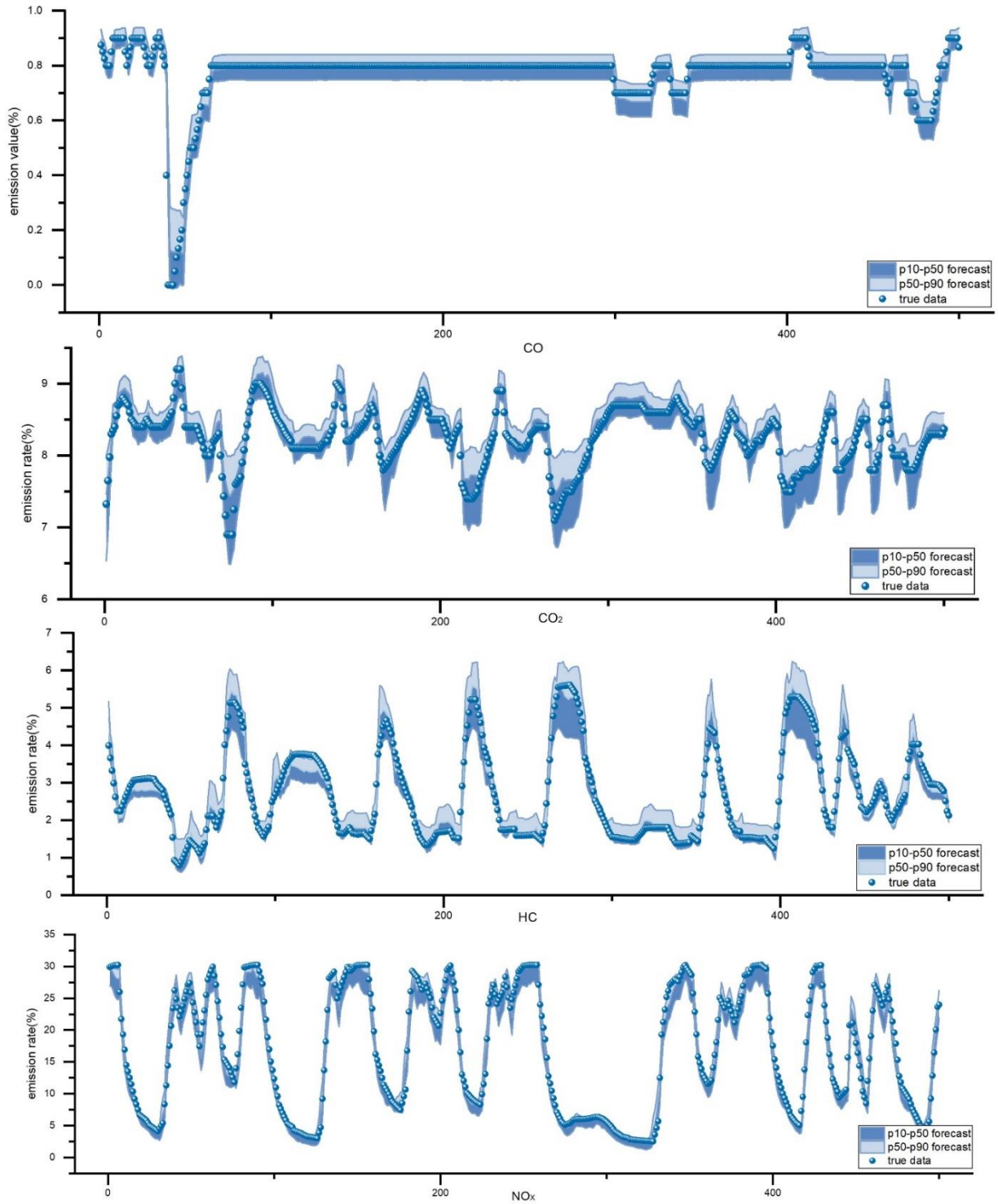


Figure 9. Comparison of TFT model exhaust emission quantile prediction results with true values.

self-adaptation of regional signals scheduling. It will reduce the exhaust emissions from buses and effectively lower them from the entire road network. In the future, with the development of intelligent transportation, the city bus system will achieve real-time perception and more information interaction, thus im-

proving operational efficiency while further saving energy and reducing exhaust emissions.

The model prediction errors for different road sections are shown in Figure 12. The TFT model performs well in predicting exhaust emissions for different road sections. CO₂, HC, and

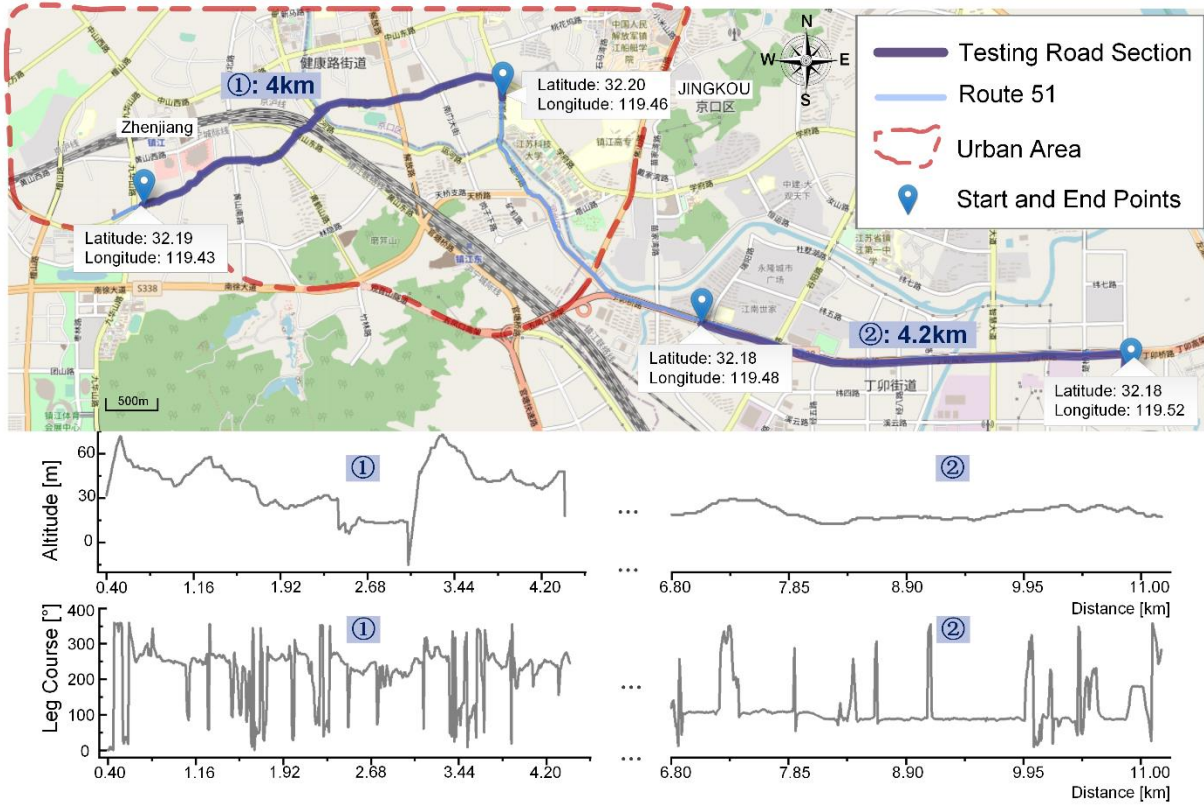


Figure 10. Location of the two test sections.

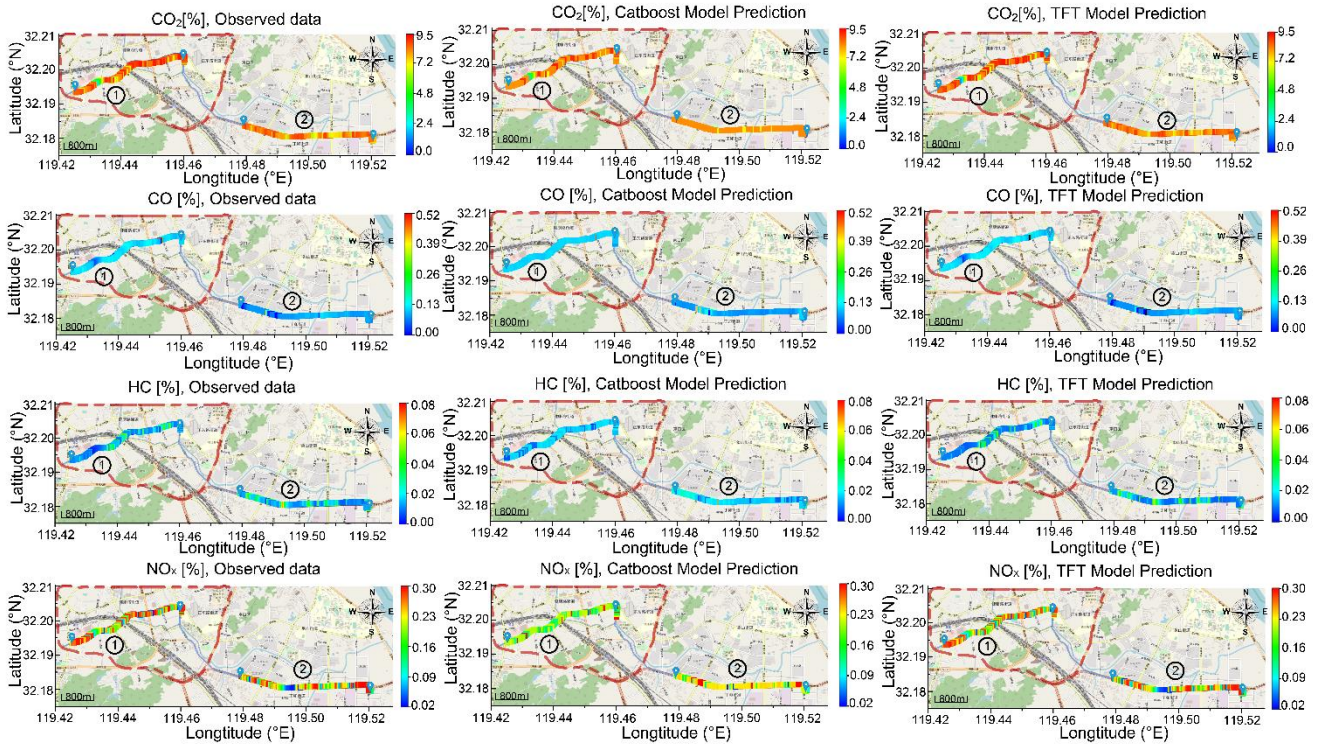


Figure 11. Comparison of observed and predicted exhaust emission values of LNG buses.

NO_x emissions are predicted with less error in section 2, mainly attributed to the simpler traffic environment and road conditions in section 2; the prediction error of CO emissions in section 1 is minor, which means that CO emissions in section 1 are more influenced by the stop-and-go driving status of the LNG bus and are more regular than those in section 2. Moreover, the LightGBM and CatBoost models show more outstanding exhaust emission prediction performance in the comparison algorithms. It is worth noting that accurate prediction of HC and NO_x emissions is more challenging, which agrees with Hu et al. (2021).

This study found that exhaust emissions are significantly higher on urban roads than on suburban roads. Urban roads have higher traffic density compared to suburban roads. Vehicles on urban roads experience more interaction with each other, leading to complex driving behaviors and frequent stop-start actions. Additionally, road conditions in urban areas are more complicated, with narrower roads and more curves. Based on these, traffic managers can arrange different fuel type buses to operate according to different operating routes and different operating hours. For example, during peak hours and in urban areas, lower-emission models (LNG or electric buses) should be arranged to operate, which can effectively reduce exhaust emissions in urban areas, and can also effectively reduce energy consumption during that time. During off-peak hours and in suburban areas, higher-emission models (such as diesel buses) can be arranged to operate, so as to effectively reduce exhaust emissions and energy consumption and meet the transportation needs of passengers as far as possible.

5.3.3. Feature Importance Analysis

Clarifying the importance of the influencing factors is crucial in light of the practical requirement to precisely predict exhaust emissions and implement low-carbon travel policies. This study exploited the variable selection networks of the TFT model to quantify the feature importance. Figure 13(a) shows the variable selection results. It can be observed that travel time (`time_on_day`) has a more significant effect on the four exhaust emissions, followed by the leg course, altitude, and acceleration factors. Probably due to the general operation of LNG buses being kept at relatively low speeds, the speed factor does not significantly affect carbon and pollutant emissions. The `is_peak` factor determines whether it is in peak hours and whether its feature weight is negligible. Peak traffic hours vary between cities, and even during peak hours, there may be brief periods of low traffic flow. Therefore, the `is_peak`, as a category-type variable in this study, cannot adequately represent the effect of traffic flow changes on exhaust emissions at different periods. The result may lead to high exhaust emission predictions during peak hours and low during off-peak hours. In addition, the impact of historical exhaust emission rates cannot be neglected.

The above features were further divided into three categories to quantify the influence of different factors: 1) traffic conditions, consisting of `time_on_day` and `is_peak`; 2) driving state, including speed and acceleration; and 3) road conditions, including leg course and altitude. Figure 13(b) shows each cat-

egory's relative feature importance. The average relative feature importance of traffic and road conditions accounted for a more significant proportion of 48.9 and 34.8%, respectively, with road conditions showing a more substantial influence on CO₂ and CO emissions. Traffic conditions have a more significant influence on HC and NO_x emissions. The above results imply that a more comprehensive perspective is necessary to accurately predict LNG buses' exhaust emissions. Therefore, to promote low-carbon travel by LNG buses, in addition to setting up bus-only lanes and improving signal control, road conditions such as road slopes can also be considered when planning bus lines.

6. Conclusions

This study focuses on the characteristics of the exhaust emissions from LNG buses. It introduces a real-time exhaust emission prediction framework for LNG buses based on the TFT model. The primary research of this paper can be summarized as follows: 1) the distribution characteristics of CO₂, CO, HC, and NO_x emissions from LNG buses were analyzed in terms of traffic conditions, driving states, and road conditions; 2) the TFT model was constructed to predict the emission rates of four exhaust gases from LNG buses, and three evaluation indicators, RMSE, MAE, and MAPE, were used to compare the prediction results with those of other advanced algorithms; 3) the emission prediction results of urban and suburban sections were compared, and the emission prediction performance of the model was further validated based on MAPE, and 4) the importance of emission features quantified by employing the variable selection networks of the TFT model. The main findings of this study can be summarized as follows.

The conclusions of this study can be concluded as follows: 1) The TFT model can efficiently learn the dependency relationship of serial data, accurately model for different operating conditions of LNG buses, and is capable of predicting peak and off-peak hours, urban and suburban road sections; through its powerful parallel computing capability, it can perform parallel operations on large scale data such as exhaust emissions, speed up training and prediction, and predict exhaust emissions in real time. 2) The TFT model uses a self-attention mechanism to take into account various factors like speed, acceleration, heading angle, altitude, etc., and learns the weights of these features. It accurately identifies the variables (traffic conditions and road conditions) that greatly impact exhaust emissions. This helps in optimizing public transport operation strategies, such as recommending suitable placement for public transport, planning bus routes, and devising traffic control strategies. For example, during peak hours and in urban areas, vehicles with lower exhaust emissions (LNG or EV) can be arranged to operate, which can effectively reduce exhaust emissions in urban areas and also effectively reduce energy consumption during this time; while during off-peak hours and in suburban areas, vehicles with higher exhaust emissions (diesel) can be arranged, which can not only reduce exhaust emissions, but also satisfy the passenger's transportation needs as much as possible.

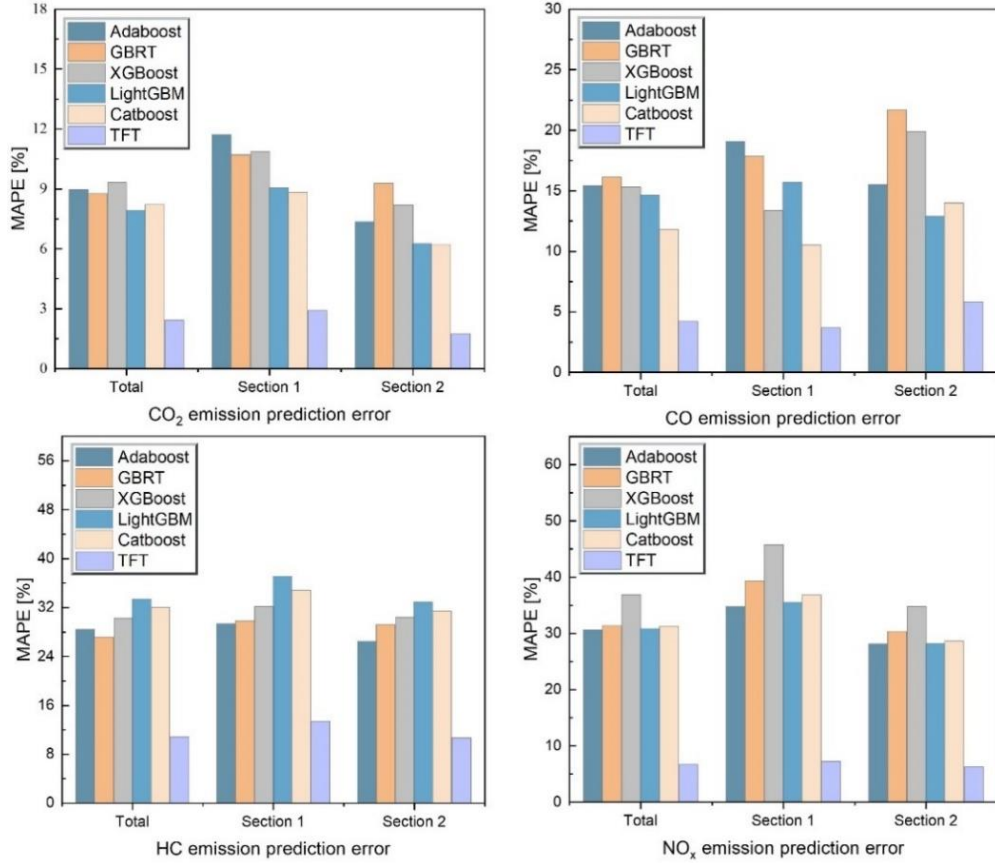


Figure 12. Comparison of the exhaust emission prediction errors for LNG buses.

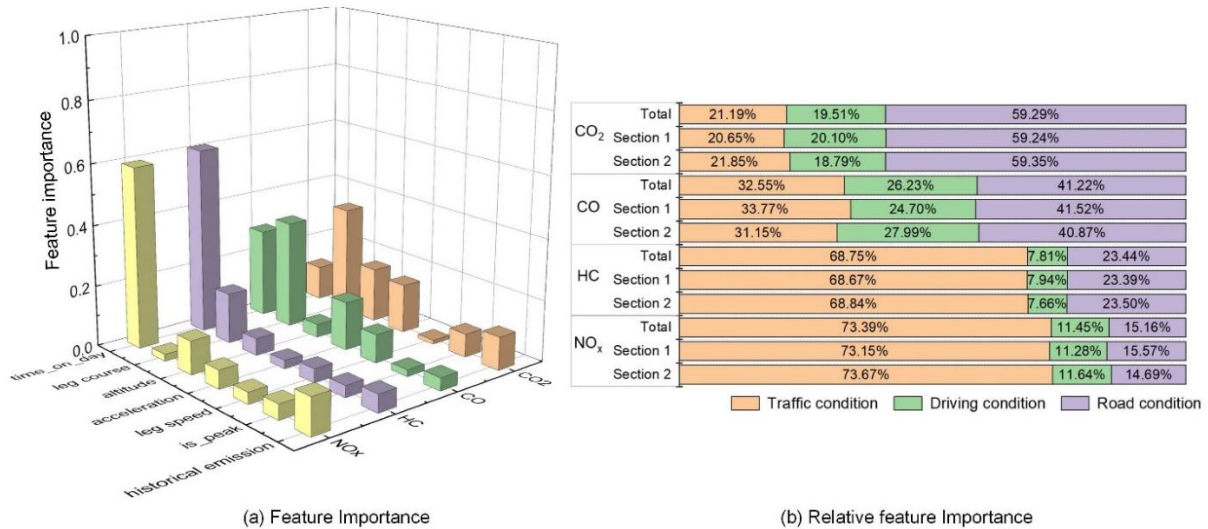


Figure 13. Feature importance of the exhaust emissions from LNG buses under different sections.

This study contributes to a sufficient understanding of the exhaust emission characteristics of LNG buses. The proposed framework can provide a reference for emission prediction of the entire

road network in cities. The above conclusions have the following main implications for urban transportation emission control policies: 1) Provide suggestions on public transport placement by

time slots and by area. Vehicles with lower exhaust emissions (LNG or electric vehicles) should be arranged to operate during peak hours and in urban sections, which can effectively reduce exhaust emissions in urban areas as well as energy consumption; 2) Guide the planning of LNG bus routes. Planning an energy-efficient and low-carbon bus route requires comprehensive consideration of road conditions, including road gradient and steering; avoiding steep uphill sections as much as possible and choosing flat routes; and choosing round intersections as much as possible when planning for curves to reduce sharp turns and braking of vehicles in order to reduce exhaust emissions. 3) Optimize traffic control strategy. Incorporating the bus operation-related features into the multi-objective optimization function, and taking the exhaust emission predicted by the TFT model in real time as the evaluation index, optimize the future traffic signal timing, stopping time of bus stops, and operation route planning, and so on, so as to improve the bus operation efficiency and reduce the level of exhaust emission.

The limitations of this study are as follows: 1) Failure to consider the effect of stopping time and number of passengers on exhaust emissions from LNG buses. The engine is idling when the bus is stopped, which can lead to the accumulation of exhaust emissions, especially NO_x; an increase in the number of passengers increases the load on the bus, which requires more power to maintain operation and increases fuel consumption, and changes in the number of passengers may also lead to changes in speed and acceleration, which can also affect exhaust emissions; 2) Failure to consider the impact of different traffic flow conditions on the exhaust emissions of LNG buses. Higher traffic densities require frequent stopping and starting of buses, which can lead to higher fuel consumption and exhaust emissions, as well as an increased likelihood of incomplete fuel combustion. Under smooth traffic flow conditions, buses operate more steadily, which can reduce fuel consumption and emission levels; 3) Failure to compare with more intelligent vehicle types, such as L3, L4, or even L5 autonomous driving buses. High-level autonomous driving is able to sense road and traffic conditions in real time and is able to plan optimal driving routes, thereby reducing exhaust emissions; high-level autonomous driving vehicles may also be equipped with advanced energy management systems that adjust operating conditions in real time to reduce exhaust emissions and fuel consumption. In the future, we will focus on the above limitations to improve the study conclusion in LNG bus exhaust emission prediction.

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