METHODOLOGY FOR THE DETERMINATION OF SPECIFIC FACTORS OF ROAD TRANSPORT EMISSION

by

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Most of the air pollution originates from combustion processes, whereby traffic is one of the most important sources. Road traffic is one of the leading factors of pollution, so determining its contribution pollution and overall emissions is very important. This study is a tool to develop a calculus method to determine the specific and annual emissions from road transport. The estimation was carried out using the methodology developed for combustion analysis. The study was based on vehicle fleet composition, fuel, and engine data, which represented the input for the combustion process simulation, while the output was combustion products. The following gases (chemical species) were included in the analysis: CO_2, CO, and NO_x. In the end, the specific emission factors, as well as bulk emission factors for urban and open road transport were derived. The results showed good agreement with the results of other authors.

Key words*: combustion, emission, pollution, traffic*

Introduction

The impact of pollutants, as a consequence of the traffic activity (CO, NO_x, CO_2, SO_x, and VOC) has been very well documented [1-6]. As estimated, in the overall balance of CO_2, vehicles participate with 10%, and in Europe with 20% of anthropogenic emissions [1, 4, 7]. Nations with rapid urbanization are becoming increasingly dependent on personal vehicle transport, which becomes a major air pollutant in urban areas [7-10]. Although the measurement of the concentration of gases itself is not demanding, a closer determination of traffic as a source is very complicated considering their stochastic nature [9-12]. For this reason, different methods for modelling emissions from traffic were suggested. Such estimates are of significant importance for more efficient management of air quality. An emission from traffic depends on numerous parameters, the most important of which are: vehicle type, engine size and type, age, fuel type, and cruising speed, all of these parameters affect the emissions. Such data, when it is sufficiently determined, can be used for building a national inventory of emissions and open a way to sustainable transport. [2, 7, 8, 13]. In recent years, there have been significant efforts to determine emissions taking into consideration engine types, engine size, and the average – cruising speed at which a vehicle is moving [14-17]. In this paper, a new approach to the traffic

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emission assessment has been suggested. Based on the vehicle's technical data (fuel type, engine size, compression ratio, *etc.*) a set of combustion equilibrium calculations was made to determine exhaust gas composition for different engine types and fuels. Furthermore, concerning fleet composition data and adopted fuel consumption for urban driving and open road scenarios, specific emission factors were determined.

Modelling of combustion for different engine types

For the determination of emission factors, a Gaseq chemical equilibrium software package was used [18, 19]. Gaseq is using the Lagrange Method of Undetermined Multipliers for minimization of the Gibbs free energy of the system to find the equilibrium state/composition. Several different types of problems can be solved using this software: composition at a defined temperature and pressure, adiabatic temperature and composition at constant pressure, composition at a defined temperature and constant volume, adiabatic temperature and composition at constant volume, adiabatic compression and expansion, and shock calculations. This makes it suitable for usage in internal combustion engine calculations where, in theory, the combustion process occurs at constant volume at Otto cycles, and constant pressure at Diesel cycles. Of all chemical species from the results of the simulation, only the main species that are in the interest for the topic were chosen to be presented: carbon-dioxide, carbon- monoxide, and NO_x.

For the purpose of analysis, vehicles were divided into three groups based on the fuel used: petrol engine vehicles, LPG vehicles, and Diesel engine vehicles. Then, based on the technical data for the typical representative of each group, typical properties of the engine – compression ratio, air to fuel ratio, and polytropic index were derived, and based on these properties, compression and combustion stroke were simulated. The pressure and the temperature after the compression stroke, and at the moment of ignition, p_i and T_i, are calculated:

$$p_\mathrm{i} = p_0 \varepsilon^n \tag{1}$$

$$T_i = T_0 \varepsilon^{n-1} \tag{2}$$

where p_0 and T_0 are assumed values of temperature and pressure after the intake stroke at the beginning of the compression stroke and ε is the compression ratio of the engine. The polytropic index n is derived from empirical correlations given in the [20, 21]:

$$n = 1.41 - \frac{100}{no} \tag{3}$$

where *no* refers to a number of revolutions of the engine shaft.

Petrol and LPG engines

For the simulation of petrol combustion, the following assumptions were made:

- petrol was assumed to be similar to isooctane and
- the fuel conditions prior to the combustion stroke were calculated on the basis of polytropic relations for internal combustion engines (ICE).

The polytropic index for compression stroke in petrol ICE n is usually between 1.35 and 1.39 and could be derived from empirical correlations [20, 21], and for a petrol ICE, assuming the value of ~2000 rpm at the cruising speed during urban driving based on the authors experience and knowledge. The value could be calculated:

$$n = 1.41 - \frac{100}{2000} = 1.36 \tag{4}$$

Similarly, for the open road the usual value is higher than ~3000 rpm, thus:

$$n = 1.41 - \frac{100}{3000} = 1.38 \tag{5}$$

The compression ratio for petrol ICE is usually around 10, whereas in modern personal vehicles, it goes up to 13 [20, 21]. According to this, the value of compression ratio which corresponds to FIAT Punto 1.2 vehicles was adopted to be $\varepsilon = 11.1$ [22]. The value of air excess coefficient is usually between 0.8 and 1.1, but at the 2/3 of power, it is closer to 1.1, so the value of 1.05 is adopted [20, 21]. Based on this data, the following parameters were determined for the mixture pressure and temperature before the ignition for urban driving:

$$p_i = 1 \times 11.1^{1.36} = 26.4 \text{ bar} \tag{6}$$

$$T_i = 273 \times 11.1^{0.36} = 649 \text{ K} \tag{7}$$

and for the open road:

$$p_i = 1 \times 11.1^{1.38} = 27.7 \text{ bar} \tag{8}$$

$$T_i = 273 \times 11.1^{0.38} = 681 \text{ K} \tag{9}$$

In theory, the combustion process for the Otto cycle is isochoric, while in reality, the ignition process starts a few degrees bTDC, and ends a few degrees after the TDC. For this reason, the maximum pressure is closer to the value of 85%, maximum 95% from the obtained theoretical pressure, fig 1, [20, 21, 23]. Therefore, after the first set of results, the constant volume equilibrium for the reduced pressure was recalculated. The equlibrium at constant volume and temperature was calculated for urban driving:

$$p^*_{max} = 0.85 p_{max} = 0.85 \times 123.3 = 104.8 \text{ bar} \tag{10}$$

$$T^*_{max} = 0.85 T_{max} = 0.85 \times 2869 = 2439 \text{ K} \tag{11}$$

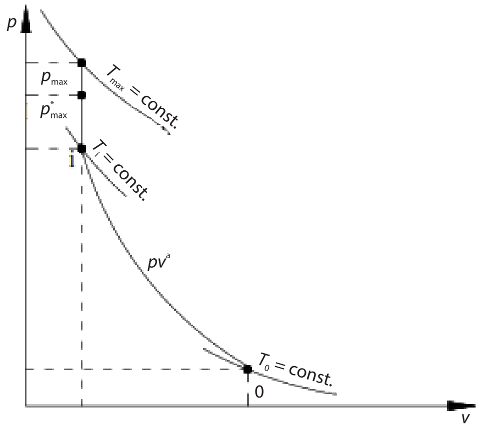

Figure 1. Characteristic parameters in *p-v* diagram for simulation of Otto cycles combustion process

and for open road:

$$p^*_{max} = 0.85 p_{max} = 0.85 \times 123.8 = 105.2 \text{ bar} \tag{12}$$

$$T^*_{max} = 0.85 T_{max} = 0.85 \times 2885 = 2452 \text{ K} \tag{13}$$

Results of emission calculations are given in tab. 1.

Table 1. Combustion products species $g_{i,p}$ for petrol engine vehicles [kg of species per kg of fuel]

Chemical species	Urban driving [kgkg^{-1}]	Open road [kgkg^{-}1]
CO_2	3.000	2.9938
CO	0.0527	0.0562
NO	0.0748	0.0768

Similarly, the combustion of LPG was modeled as the combustion of propane. The equlibrium at constant volume and temperature was calculated for urban driving at:

$$p^*_{\max} = 0.85 p_{\max} = 0.85 \times 120.6 = 102.5 \text{ bar} \tag{14}$$

$$T^*_{\max} = 0.85 T_{\max} = 0.85 \times 2855 = 2427 \text{ K} \tag{15}$$

and for open road:

$$p^*_{\max} = 0.85 p_{\max} = 0.85 \times 123.8 = 105.2 \text{ bar} \tag{16}$$

$$T^*_{\max} = 0.85 T_{\max} = 0.85 \times 2869 = 2439 \text{ K} \tag{17}$$

The results for combustion of m = 1 kg of fuel are presented in tab. 2.

Table 2. Combustion products species $g_{i,l}$ for LPG engine vehicles [kg of species per kg of fuel]

Chemical species	Urban driving [kgkg^{-1}]	Open road [kgkg^{-1}]
CO_2	2.9172	2.9127
CO	0.0489	0.05175
NO	0.0754	0.07706

Diesel engines

The diesel ICE was simulated similarly to petrol engines. The following characteristics were adopted for diesel ICE [20-22]:
- the compression ratio which is usually between 12 and 20 was adopted as 17.6 which corresponds to FIAT Punto vehicle,
- the exponent of polytrope 1.36 for urban driving,
- the exponent of polytrope 1.38 for open road driving,
- the combustion process is isobaric, amd
- the air excess coefficient is equal to 1.5.

According to this, and eq. (1)-(3) the initial temperature was set to 766 K, and pressure to 49.4 bar for urban driving, while the initial temperature was set to 805 K, and pressure to 51.9 bar for an open road driving.

In contrast to the theoretical Otto cycle, the combustion process in the Diesel cycle is isobaric, while during the combustion, the pressure after the autoignition raises between 1.3 and 3.5 times [20, 21]. Thus, after the first set of results, the equilibrium at the constant pressure increased 1.825 times and the second iteration was calculated, fig. 2.

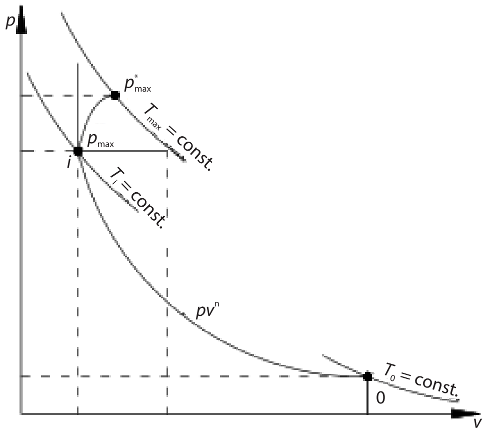

Figure 2. Characteristic parameters in *p-v* diagram for simulation of Diesel cycles combustion process

The equlibrium at constant volume and temperature was calculated for urban driving at:

$$p^*_{\max} = 1.825 p_{\max} = 1.825 \times 49.4 = 90.1 \text{ bar} \tag{18}$$

$$T_{\max} = 2191 \text{K} \tag{19}$$

and for open road:

$$p^*_{\max} = 1.825 p_{\max} = 1.825 \times 51.9 = 94.7\,\text{bar} \tag{20}$$

$$T_{\max} = 2222\,\text{K} \tag{21}$$

The obtained values for the products composition after the combustion of 1 kg of fuel are presented in the following tab. 3. The data is in good agreement with the results presented in papers [24, 25].

Table 3. Combustion produst species $g_{\text{i,d}}$ for diesel ICE vehicles [kg of species per kg of fuel]

Chemical species	Urban driving [kgkg^{-1}]	Open road [kgkg^{-1}]
CO_2	3.0748	3.0734
CO	0.00468	0.00560
NO	0.17186	0.18361

Calculation of specific emission factors

For the determination of specific emission factors, the following assumtions were adopted on the basis of experience and technical data presented in [22]:
- in urban driving the petrol fuel consumption is 10 L per 100 km, or 7.66 kg per 100 km,
- in open road driving the petrol fuel consumption is 8 L per 100 km, or 6.13 kg per 100 km,
- in urban driving the LPG fuel consumption is 11.5 L per 100 km, or 6.44 kg per 100 km,
- in open road driving the LPG fuel consumption is 9.2 L per 100 km, or 5.15 kg per 100 km,
- in urban driving the Diesel fuel consumption is 7.7 L per 100 km, or 6.7 kg per 100 km, and
- in open road driving the LPG fuel consumption is 5 L per 100 km, or 4.35 kg per 100 km.

According to this assumptions, and results presented in tabs. 1-3, the following specific emission factors are obtained:

$$e_{\text{i,f}} = g_{\text{i,f}} F \times \frac{1000\ \text{g/kg}}{100\,\text{km}} \tag{22}$$

and the results are presented in tab. 4.

Table 4. Specific emission factors for different engine types

	Urban driving [gkm^{-1}]	Open road [gkm^{-1}]
Petrol engines		
$e_{CO_2,\text{pet}}$	229.8	183.8
$e_{CO,\text{pet}}$	4	3.4
$e_{NO_x,\text{pet}}$	5.7	4.7
LPG engines		
$e_{CO_2,\text{LPG}}$	187.9	150
$e_{CO,\text{ LPG}}$	3.2	2.7
$e_{NO_x,\text{ LPG}}$	4.9	4.0
Diesel engines		
$e_{CO_2,\text{D}}$	205.8	133.7
$e_{CO,\text{ D}}$	0.3	0.2
$e_{NO_x,\text{ D}}$	11.5	8.0

According to the data in 2018, there were 1999771 personal vehicles, 39.3% of which are petrol engines, 47.8% are Diesel engines, and the remaining 12.9% are LPG engines [26]. Based on this data and specific emissions for different engine technologies, it is feasible to determine the bulk emission factor for vehicles in the Republic of Serbia, tab. 5:

$$E_{\mathrm{i}} = \sum e_{\mathrm{i,f}} \mathrm{share}_{\mathrm{f}} \tag{23}$$

Table 5. Bulk emission factors for vehicles in the Republic of Serbia

	Urban driving [gkm^{-1}]	Open road [gkm^{-1}]
$E_{\mathrm{CO2,pet}}$	212.9	156.6
$E_{\mathrm{CO,\,pet}}$	2.1	1.8
$E_{\mathrm{NO}x\mathrm{,\,pet}}$	8.4 (0.84)	6.2 (0.62)

Calculation of specific emission factors

According to the work of Samaras *et al.* [16], the bulk emission factor for different countries in Europe could be calculated as functions of fuel consumption. According to their research and adopted assumptions for the newly independent states in East Europe, the results for 2002 are presented in the following tab. 6.

Table 6. Bulk emission factors for vehicles in newly independent states in East Europe [16]

	Urban driving [gkm^{-1}]	Open road [gkm^{-1}]
Petrol engines		
$E_{\mathrm{CO_2,pet}}$	208.3	166.7
$E_{\mathrm{CO,\,pet}}$	16.98	13.6
$E_{\mathrm{NO}_x\mathrm{,\,pet}}$	2.17	1.74
Diesel engine		
$E_{\mathrm{CO_2,D}}$	207.0	134.4
$E_{\mathrm{CO,\,D}}$	8.5	9.6
$E_{\mathrm{NO}_x\mathrm{,\,D}}$	7.8	0.5

In general, the obtained results for CO_2-specific emission factors are in good agreement with emission factors for newly independent states; however, there is a significant gap in results for CO and NO_x-specific emission factors, but one should note that the results for specific countries differ significantly. For example, the specific emission factor for CO is almost three times higher in Romania in comparison with Slovenia, tabs. 7 and 8, and results for CO specific emission factors in Slovenia are in a good agreement with the obtained results.

Furthermore, Joumard *et al.* [17] have tested a group of different personal vehicles samples of gasoline or diesel cars, with or without catalytic converters and presented the overall results for specific emission factors for different driving regimes. This results for CO_2 and CO emission factors are in a good agreement with the current, tab. 9.

In their research, Ayede *et al.* [6] gave the bulk specific emission factors for urban vehicle driving in a Serbian city Niš, which are slightly higher for CO_2 and CO. However, it should be noted that these results apply to the overall fleet of vehicles including buses and

Table 7. Calculated bulk emission factors in Romania [16]

	Urban driving [gkm^{-1}]	Open road [gkm^{-1}]
Petrol engines		
$E_{CO_2,pet}$	311.0	248.9
$E_{CO,\,pet}$	20.7	16.6
$E_{NO_x,\,pet}$	1.5	1.2
Diesel engine		
$E_{CO_2,D}$	268.1	164.2
$E_{CO,\,D}$	0.4	0.26
$E_{NO_x,\,D}$	0.8	0.54

Table 8. Calculated bulk emission factors in Slovenia [16]

	Urban driving [gkm^{-1}]	Open road [gkm^{-1}]
Petrol engines		
$E_{CO_2,pet}$	312	253.8
$E_{CO,\,pet}$	6.5	5.2
$E_{NO_x,\,pet}$	0.67	0.5
Diesel engine		
$E_{CO_2,D}$	270	176
$E_{CO,\,D}$	0.2	0.2
$E_{NO_x,\,D}$	0.9	0.6

trucks. The main difference in the results is in specific factors for NO_x emission, and the main reason for this is the existence of a catalyst that reduces up to 90% of NO_x emissions in the environment [27, 28]. So, if we simply multiply the NO_x specific emission factors with 10%, the obtained results presented in brackets in tab. 5 are in a good agreement with results for Slovenia and research of Joumard *et al.* [17].

Table 9. Samples of gasoline or diesel cars, with or without catalytic converters [17]

	Urban driving [gkm^{-1}]	Open road [gkm^{-1}]
$E_{CO_2,pet}$	258.3	149.3
$E_{CO,\,pet}$	3.3	1.18
$E_{NO_x,\,pet}$	0.35	0.33

Uncertainty analysis

For the error analysis, the specific bulk emission in urban transport was chosen. The results are presented in the following tab. 10.

Table 10. Uncertainty analysis for specific emission factors

Authors	E_{CO_2}	E_{CO}	E_{NO_x}
[17]	258.3	3.3	0.35
[16]	330	9.7	0.76
Current research	212.9	2.1	0.84
Averagde	267.07	5.03	0.65
Uncertanty	22.6%	158.9%	25.6%

The obtained uncertainty ranges from 22.6% to 159%. However, the uncertainty presented in the tab. 10 is in good agreement with uncertainty presented in the report [29], and the results obtained in the research for specific emission factors for CO_2 and NO_x are similar for all the authors. The greatest disparity, as it could be noted, arises in the emission factors for CO, but there is also a good agreement between emission factors for CO obtained in the presented research, and the research of Joumard *et al* [17]. In comparison the paper presented by Joumard *et al.* [17] the difference for specific emission factor for CO is 28.6% in value, which is close to results for both specific emission factors for CO_2 and NO_x.

Conclusion

This paper presents a novel method for determining emissions from road transport. Based on personal vehicle technical data, a set of combustion simulations was run for different engine categories depending on fuel, and products of chemical combustion per kg of fuel were obtained. According to this data and the assumed fuel consumption, specific vehicle emissions were calculated in kg and per km for urban and open road driving. On the basis of this methodology and results, it is possible to do an assessment of emissions from road transport even only on basis of statistical data as annual fuel consumption, or average annual mileage of a vehicle.

Nomenclature

E – bulk emission factors, [gkm^{-1}]
e – specific emission factors, [gkm^{-1}]
F – fuel consumption per 100 km, [kg]
g – combustion species emission per kg of fuel, [kgkg^{-1}]
no – revolutions per minute, [min^{-1}]
p – pressure, [bar]
T – temperature, [K]

Greek symbol

ε – compression ratio, [–]

Subscripts

i – co-ordinate
f – fuel type

Reference

[1] Nejadkoorki, F., *et al.*, An Approach for Modelling CO_2 Emission from Road Traffic in Urban Areas, *Science of the Total Environment*, *406* (2008), 1-2, pp. 269-278
[2] Machado, A., *et al*., Air Emissions Inventory of the Public Transport in Maracaibo Municipality – Part I: Passenger Car, *Rev. Téc. Ing. Univ. Zulia*, *27* (2004), 3, pp. 202-209
[3] Živković, P., *et a*l., Air Pollution Estimation in The City of Niš Territory, *Proceedings*, International Symposium Power Plants 2010, Vrnjačka Banja, Serbia, 2010, pp. 248-251
[4] Nikolaoua, K., *et al*., Traffic and Air Pollution Temporal Evolution in the City of Serres, Greece, *Journal of Environmental Protection and Ecology*, *10* (2009), 2, pp. 320-326
[5] Živković, P., *et al*., Local Traffic Intensity Influence on Air Quality in Niš, *Proceedings*, 24th International Conference on Efficiency, Cost, Optimization, Simulation and Environmental Impact of Energy Systems – ECOS 2011, Novi Sad, Serbia, 2011, pp. 2230-2238
[6] Ayed, S., *et al*., A Specific Approach for Estimating Traffic-Induced Urban Pollution, *Pol. J. Environ. Stud*., *24* (2015), 6, pp. 2739-2744
[7] Nesamani, K. S., Estimation of Automobile Emissions and Control Strategies in India, *Sci. Total Environ*., *408* (2010), 8, pp. 1800-1811
[8] Du, Y., Geng, Y., Sun, L., Simulation Model Based on Monte Carlo Method for Traffic Assignment in Local Area Road Network, *Front. Archit. Civ. Eng. China*., *3* (2009), 2, pp. 195-203
[9] Sturm, P., *et al*., Application of Computational Methods for the Determination of Traffic Emissions, *Air Waste Manage Assoc*, *47* (1997), 11, pp. 1204-1210
[10] Ćirić, I. T., *et al*., Air Quality Estimation by Computational Intelligence Methodologies, *Thermal Science*, *16* (2012), Suppl. 2, pp. S493-S504
[11] Živković, P., *et al*., Specific Approach for Continuous Air Quality Monitoring, *Hemijska industrija*, *66* (2012), 1, pp. 85-93
[12] Andre, M., Hammarstrom, U., Driving Speeds in Europe for Pollutant Emissions Estimation, Transportation Research – Part D: *Transport and Environment*, *5* (2000), 5, pp. 321-335
[13] Manojlović, A. V, *et al*., Fleet Renewal: An Approach to Achieve Sustainable Road Transport, *Thermal Science*, *15* (2011), 4, pp. 1223-1236
[14] Washburn, S., *et al*., Statistical Modelling of Vehicle Emissions from Inspection/Maintenance Testing Data: An Exploratory Analysis, Transportation Research – Part D: *Transport and Environment*, *6* (2001), 1, pp. 21-36

[15] Nesamania, K. S., *et al.*, Estimation of Vehicular Emissions by Capturing Traffic Variations, *Atmospheric Environment*, *41* (2007), 14, pp. 2996-3008
[16] Samaras, Z., *et al*., Air Pollutant Emission Inventory Guidebook 2019 – Update Oct. 2021, Europian Environmental Agency, Copenhagen, Denmark, 2021
[17] Joumard, R., *et al*., Influence du cycle de conduite sur les emissions unitaires de pollutants des voitures particulieres (in French). INRETS Report, No. LTE 9902, Bron, France, 1999
[18] ***, http://www.gaseq.co.uk/
[19] Tomić, M., *et al*., The Pollutant Emissions Assessment from Personal Vehicles in the Republic of Serbia, *Proceedings*, 1st International Conference on Advances in Science and Technology, Herceg Novi, Montenegro, 2022
[20] Živković, M. C., *Motori sa Unutrašnjim Sagorevanjem – I Deo*, *Teorija Motora*, Mašinski Fakultet Beograd, Beograd, SFRJ, 1988
[21] Stefanović, A., Aković, R., *Motori sa Unutrašnjim Sagorevanjem Repetitorijum*, Mašinski Fakultet Niš, Niš, SRJ, 1996
[22] ***, https://www.automanijak.com/modeli/fiat/67/fiat-grande-punto-2005#gsc.tab=0
[23] Tomić, M, *et al.*, Closed Vessel Combustion Modelling by Using Pressure-Time Evolution Function Derived from Two-Zonal Approach, *Thermal Science*, *16* (2012), 2, pp. 561-572
[24] Resitoglu, I. A., *et al*., The Pollutant Emissions from Diesel-Engine Vehicles and Exhaust Aftertreatment Systems, *Clean Technology and Environmental Policy*, *17* (2015), Jan., pp. 15-27
[25] Muncrief, R., The NO_x Emissions from Heavy-Duty and Light-Duty Diesel Vehicles in the EU: Comparison of Real-World Performance and Current Type-Approval Requirements, International Council on Clean Transportation, Washington DC, USA, 2021
[26] Manojlović, A., *et al*., Study on Assessment of Pollutant Emissions from Road Transport on National Roads of the Republic of Serbia 2016-2018, Intico Ltd., Belgrade, Serbia, 2020
[27] Heimrich, M. J., Demonstration of Lean NO_x Catalytic Converter Technology on a Heavy-Duty Diesel Engine, *Journal of Fuels and Lubricants*, *106* (1997), 4, pp. 282-292
[28] ***, https://ipa-news.com/index/pgm-applications/automotive/catalytic-converters/by-how-much-do-they-reduce-pollution.html?PHPSESSID=1eab3fd396c7cad1bbfe08bca4fae038
[29] Geilenkirchen, G., *et al*., Methods for Calculating the Emissions of Transport in the Netherlands, Report No. 4616, Netherlands Environmental Assessment Agency, Hague, The Netherlands, 2021

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