Ultra-low emissions with OME at the CI engine – Implementation and potential for reduction of the immission level

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Introduction

Although the continuous tightening of the European exhaust emission legislation has reduced inner-city immissions in the past, the currently permissible limits are still being exceeded in certain metropolitan areas. In the light of emission levels of internal combustion engines that are technologically achievable today, the question of their impact on immission levels is gaining importance increasingly. For future powertrain development it is of interest, to what extent future limits can be reached with currently available technology and to additionally quantify their boundary values.

Compliance to future CO_2 targets in the transport sector solely on the basis of progress in engine technology seems unrealistic in consideration of the background of steadily increasing vehicle fleet kilometer performance. Provided that the provision of energy for electrically powered vehicles is associated with little or no CO_2 release, CO_2 fleet emissions can be reduced with electric powertrains effectively. However, challenges such as the usable power densities of current battery systems and corresponding high vehicle weights, recyclability and the use of rare earths remain.

Although a reduction in CO_2 emissions can be achieved with classic combustion engines by means of electrification, the challenges of electric vehicles remain for hybrid powertrains as well. Another possibility for CO_2 reduction is given by the fuel path, as during the synthesis of the fuel CO_2 is being bound. CO_2 release during subsequent combustion is therefore to be assessed as CO_2 neutral, as long as the production process is also CO_2 neutral. The main advantages of this approach are that well established and highly developed technology can be used further, customer handling is easy and accepted and finally no additional infrastructure is needed. All in all, a significant CO_2 reduction could be achieved very quickly and sustainably in this way.

One representative of these synthetic fuels is the group of oxymethylene ethers (OME). Due to its high oxygen content and no direct, intermolecular carbon bonds, it burns much cleaner and more efficiently as conventional fuel. In combination with currently available exhaust aftertreatment components as well as an adaptation of the combustion process on a conventional series production engine, the potential for a CO_2-neutral drive with minimal pollutant emissions is investigated. In connection with the influence of exhaust gas emissions on immission levels, it is also shown what contribution engine concepts of this type can make to reduce pollutants in metropolitan areas and what immission level they can be classified into. The results shown here were obtained within the framework of a project whose aim was to demonstrate the potentials of the technologies investigated.

Emission – Immission interaction and quantification

In the past, European automotive emissions legislation has become increasingly strict. Despite all efforts, some cities do not comply with the immission limits in force. In order to develop a better understanding of the interaction between emission and immission and to be able to quantify this correlation, an example is defined here and a corresponding emission-immission model is developed and presented.

If the situation in Germany is considered as an example for industrialized countries, it can be seen that the traffic-related emissions of various species have been decreasing continuously in recent years although annual vehicle fleet mileage has increased [1] [2]. The Air Quality Directive 2008/50/EC currently defines immission limits which, contrary to the decreasing emissions in metropolitan areas, are in some cases significantly exceeded. However, the situation is contradictory. While the majority of measuring stations are permanently in compliance with the applicable limits, there are also sites where the immission limits are continuously exceeded. The common factor of all stations with high violations of the limits is their position in close proximity to a street [3].

In order to meet the central objective of the Federal Immission Control Act, the aim must be to keep the emission-related exposure on the population as low as possible. Under this premise, a definition was made within the framework of the project presented here, within which future development goals can be classified on the basis of the level of immissions. The core idea behind this concept is the question of the contribution of the vehicle fleet to local immission levels. In the following, three terms of immission levels are defined, which are used to evaluate and classify the results obtained in the context of the underlying project.

Zero Impact Vehicle	Emission of the vehicle fleet has no influence on the immission measurement result in a specific measurement scenario (in the range of the natural fluctuation of the background)
Leveling Vehicle	Emission of the vehicle fleet reduces the immission result in specific measurement scenario in and near the driving zone
SubZero Vehicle	Emission of the vehicle fleet reduces the immission result in specific measurement scenarios and also reduces the background level

The idea of this definition and its immission impact can be illustrated by an exemplary vehicle fleet: Battery electric vehicles cannot change the immission level as they do not induct air and process it thermodynamically. Thus, the concentration of pollutants is the same in front and behind the vehicle. Within the above definition, it is therefore equivalent to a Zero Impact Vehicle. A Leveling Vehicle reduces the given concentration in the driving zone, but does not fall below the background level in the metropolitan area. This is only relevant as long as the driving zone contains increased concentrations due to high emission sources and thus represents a bridging technology. SubZero Vehicles are characterized by lowest raw emissions combined with a highly efficient exhaust gas aftertreatment (EGA) systems, so the pollutant concentration drops below the metropolitan immission level at a specific immission monitoring point and thus the immission level is decreased in the long term. For particulate emissions this seems already feasible today [4], but for nitrogen dioxide emissions the corresponding concentrations are challenging.

The evaluation within a defined measurement scenario, e.g. at a certain monitoring point, is highly dependent on the specific boundary conditions, which is why this aspect is also part of the definition. Measured immissions are dependent on factors such as wind, rain, temperature and radiation energy. These factors can vary significantly from one place to the other. This is most likely one of the main reasons for such a large scatter of the results when limit values are exceeded [5]. As the background immission level is not constant but part of the definition at the same time, also the immission class itself is not fixed. It is continuously decreasing over time in the respective scenario. If the measurement station at Darmstadt Hügelstraße is taken as an example, the natural fluctuation of the rural immission background within a ten-year period ranges in the order of 5 – 10 µg/m³ (≈ 3 – 5 ppb) NO_2 [6].

In order to connect the immission impact of the introduced definition to todays vehicle emission quantities, an exemplary scale was derived to quantify an estimation of current and future emission levels, illustrated in Figure 1.

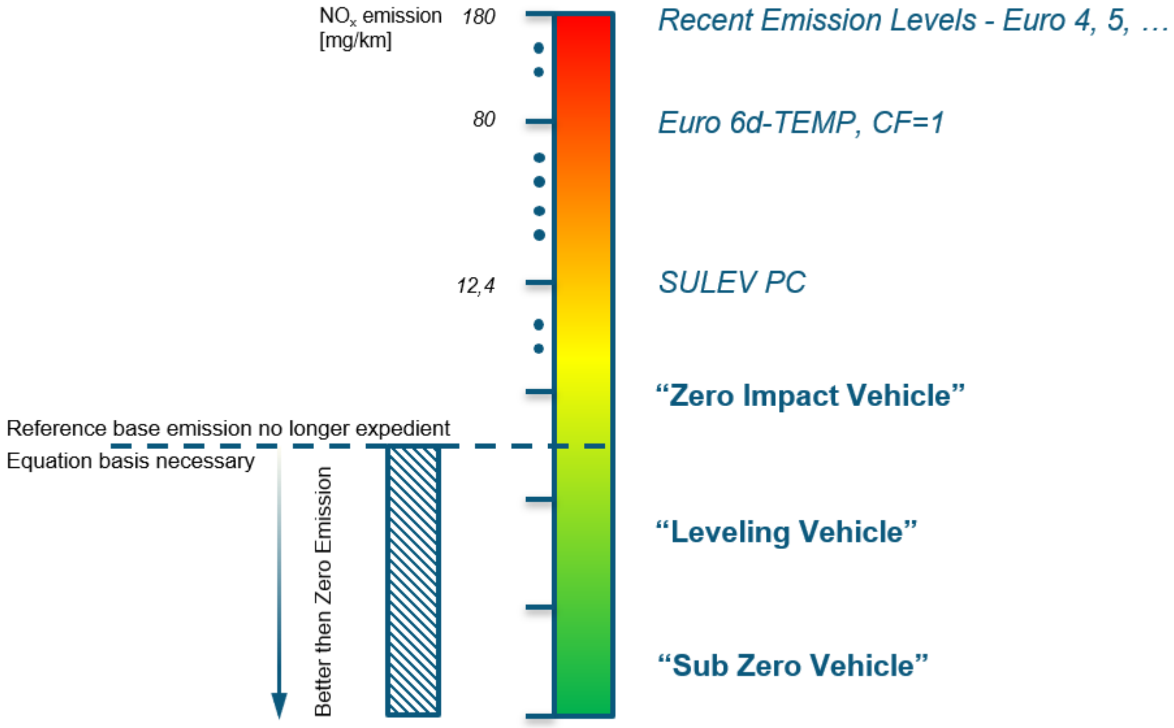

Figure 1: Classification of lowest emission vehicles compared to an estimation of corresponding specific tailpipe emission levels

If tailpipe emissions can be realized to the extent shown here, it is questionable, weather the impact shall further be regulated or investigated by the output of an emitter. For future legislation one approach could be equation based, on the sum over the system boundary of a vehicle. A certain concentration is entering, another concentration leaving the object under investigation. Inside the system boundary, statistically validated diluting effects are considered and the vehicle's immission impact is derived directly. Measurements conducted at VKM besides the content of the project presented here indicate a dilution factor of tailpipe emission to street side concentrations in the magnitude of 100. In a first stage, the tailpipe to driving zone concentration dilution factor ranges in a magnitude of a factor of 10.

To quantify the influence of today’s vehicle fleet's emissions on the measured immission at the measuring station under different boundary conditions, an empirical model is used to calculate the additional pollution caused by traffic for the Darmstadt Hügelstraße measuring station at half-hourly resolution. The selected measuring station is among the ones with highest exceedings of the yearly immission limit value in Germany [7]. Figure 2 shows the calculation process in the simulation.

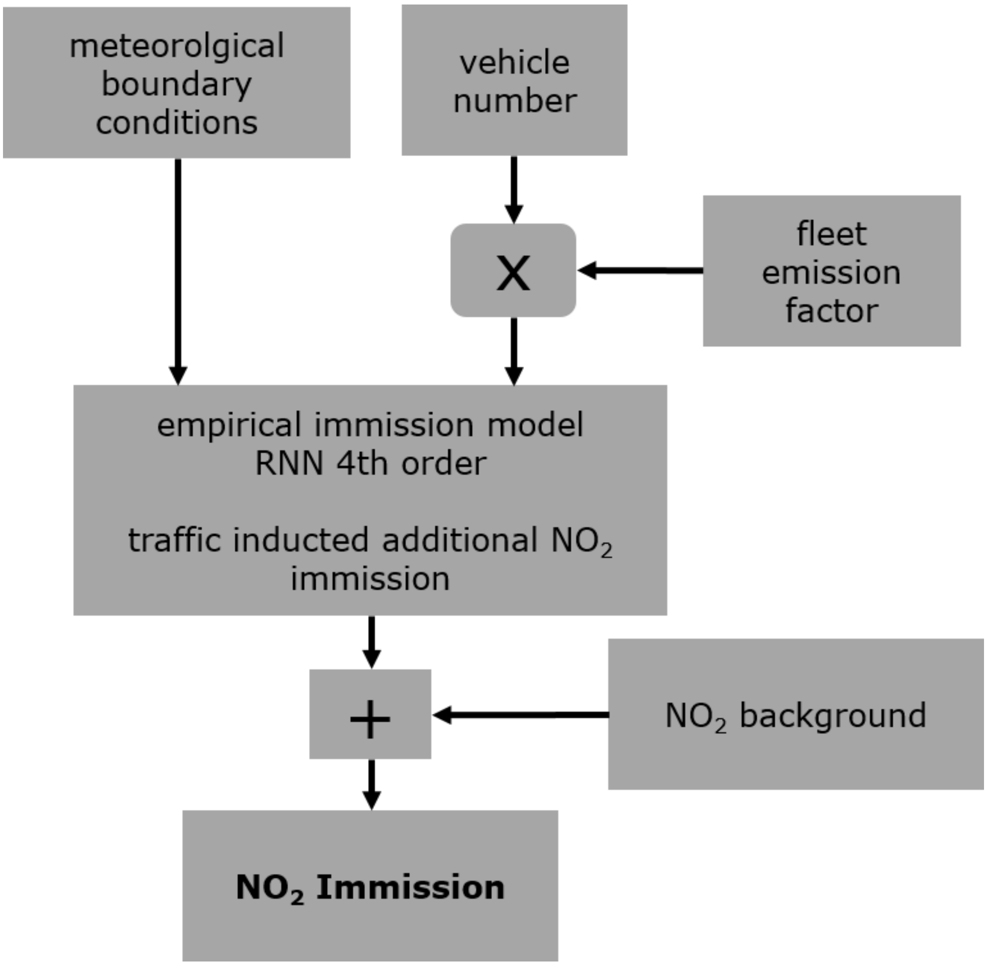

Figure 2: Schematic overview of the model structure for inner city immissions

The database of the model is based on meteorological measurement data, the measured immissions and the vehicle fleet passing the measuring station, which is additionally divided into different vehicle classes. This data was provided by the Hessian Agency for Nature Conservation, Environment and Geology (HLNUG). In order to assign an emission to the vehicle fleet so that it can be correlated to the measured immission, the emission factors from HBEFA[1] 4.1 are used. The model is created in form of a 4th order neural network, which outputs the NO$_2$ immission in addition to the urban background. With the help of the model, it is possible to investigate the effects of arbitrarily designed vehicle fleets on the immission in terms of both number of vehicles and emission factor. The meteorological boundary conditions can also be chosen arbitrarily or repeated from a reference year. For the results presented here, the model was validated on the reference year 2018 and all parameters except for emissions and fleet composition were fixed. As the NO$_2$ immission background is implemented based on existing measurement data, it is not possible to quantify a potential reduction of the immission background due to lowered emission levels of the vehicle fleet.

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[1] HBEFA: HandBuch für EmissionsFAktoren des Straßenverkehrs, published by INFRAS

Experimental setup

The main objective of the project was the direct comparison of a series production engine operated with conventional petrol station diesel and pure OME_{3-6} to identify the maximum potential for lowest pollutant emissions. The used OME_{3-6} mixture consists of ~ 47% OME_3, ~ 30% OME_4, ~ 17% OME_5 and ~ 6% OME_6. OME_{3-6} has highly comparable properties to diesel fuel. Even though, its density and kinematic viscosity do not comply with the norm, whereas the lubricity (HFRR) remains within the permitted range. As expected, the lower calorific value is lower due to the bound oxygen. [8][9]

For the investigations within the scope of the project, a series production engine with compression ignition was used. No component adjustments were made to the engine under test. The data of the engine control unit (ECU) basically corresponds to the series production status. Within a limited range, certain quantities were accessible for modifications such as the injected fuel quantity, timing parameters of the fuel injection, the amount of recirculated exhaust gas (EGR rate) and the boost pressure. All other parameters are, as far as possible, kept constant or at least not actively changed over the different measurement series. Table 1 shows the characteristic properties of the engine.

Table 1: Characteristic parameters of the engine under test

Parameter	Unit	Value
Max. Engine Speed	rpm	5000
Max. Power	kW	173
Max. Torque	Nm	480
No. of cylinders	-	4
Displacement	cm^3	1969
Bore / Stroke	mm	82 / 93.2
Compression ratio	-	15.8:1

In the first test series of the project, the series production exhaust gas aftertreatment system was installed, but without a diesel particulate filter. The focus of these investigations was to initially demonstrate the potential of pure OME operation. In a next step the exhaust gas aftertreatment system was adapted for maximum efficiency, consisting of a 2 kW electrically heated catalyst (EHC), a diesel oxidation catalyst (DOC), a SCR-catalyzed diesel particulate filter (sDPF) as well as two selective catalytic reduction catalyst (SCR). One is close coupled to the engine exhaust, the other one in a distance similar to an underfloor catalyst of a car. The schematic layout of the exhaust gas aftertreatment system is shown in Figure 3.

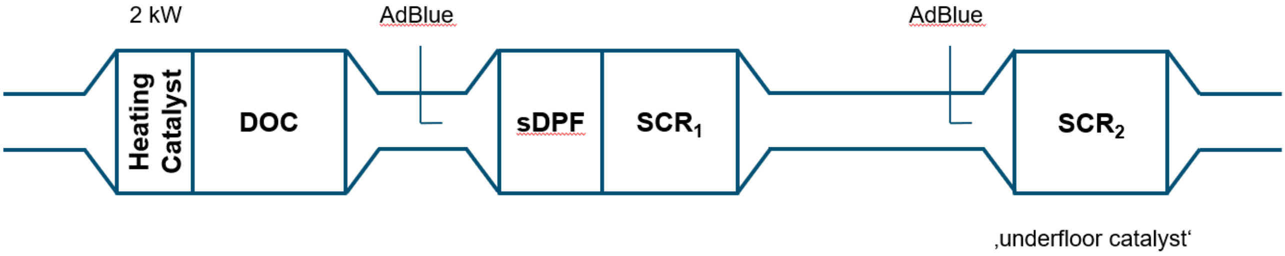

Figure 3: Component overview of used exhaust aftertreatment system

In terms of availability and technology level, series components are used for the exhaust system. Perspectively it may be possible to omit or reduce individual components. However, in order to prove maxima of this potential analysis, all exhaust gas components are implemented. The use of OME leads to lower exhaust gas temperatures in most areas of engine operating points. In order to compensate for this effect, especially at low engine loads, no engine-side heating measures are implemented (e.g. via late fuel injection) but the heating catalyst is used to ensure optimum conversion conditions throughout the entire engine map. The AdBlue dosing (urea-water solution) serves to provide ammonia for the SCR reaction on the sDPF and the SCR catalysts.

Extensive measurement technology is used within the scope of the project and the test program. The measurement of legally regulated pollutant emissions is carried out with an AVL AMA i60. Legally unregulated emissions, e.g. methane, formaldehyde and unburned OME, are measured by an AVL SESAM i60 FT. For particle measurement a PMP-compliant AVL 489 Particle Counter (particle number) and a Cambustion DMS 500 (Particle number and size distribution) are used. Fuel consumption is measured using an AVL FuelExact. The fuel temperature is conditioned to 20°C. For combustion analysis high pressure sensors are implemented in the cylinder and the injection is monitored with injector current measurement. Air path, engine and exhaust path are further fully equipped with sensors for temperature and pressure measurement.

Four representative operating points are defined for the investigations within the research project. They are derived by binning engine operating points in speed and torque, based on a selection of RDE trips that were carried out at VKM in the past. Only vehicles that were equipped with comparable engines are considered. Irrelevant operating states and operating points such as idling, shifting and coasting are excluded from the analysis. The corresponding operating points are summarized in an overview in Table 2.

Table 2: Definition of investigated operating points

Operating Point	**Engine Speed**	**Engine Torque**	**Engine Power**
	rpm	Nm	kW
OP 1	1250	37	6.6
OP 2	1500	47	9.4
OP 3	1750	116	22.0
OP 4	2250	130	33.0

During the measurements the operating points are kept constant for all fuels (diesel and pure OME) and the various engine applications. The adjustment of load (engine torque) is performed by increasing the injected fuel quantity. The injection pattern itself is not changed. In addition, various application goals are pursued. In a first optimization loop, the lowest possible NO_x raw emissions are represented by a maximum increase of EGR rate. In a next step, further parameters like combustion efficiency and low engine out emissions of other species are included. A moderate EGR rate is applied and the center of combustion is shifted towards its optimum to compensate for the longer injection time. Based on this last application stage, an investigation is carried out with the EGA system described above. In operating points critical in regard to low exhaust gas temperatures, the EHC is activated. The results of these final investigations are presented in this paper.

Results

Within the scope of the measurement campaign the operating points presented in the previous section are measured. Figure 4 lists the results of the legally regulated species in the exhaust gas, measured with AMA i60, both as concentration for direct comparison of the ambient air concentration and power-specific.

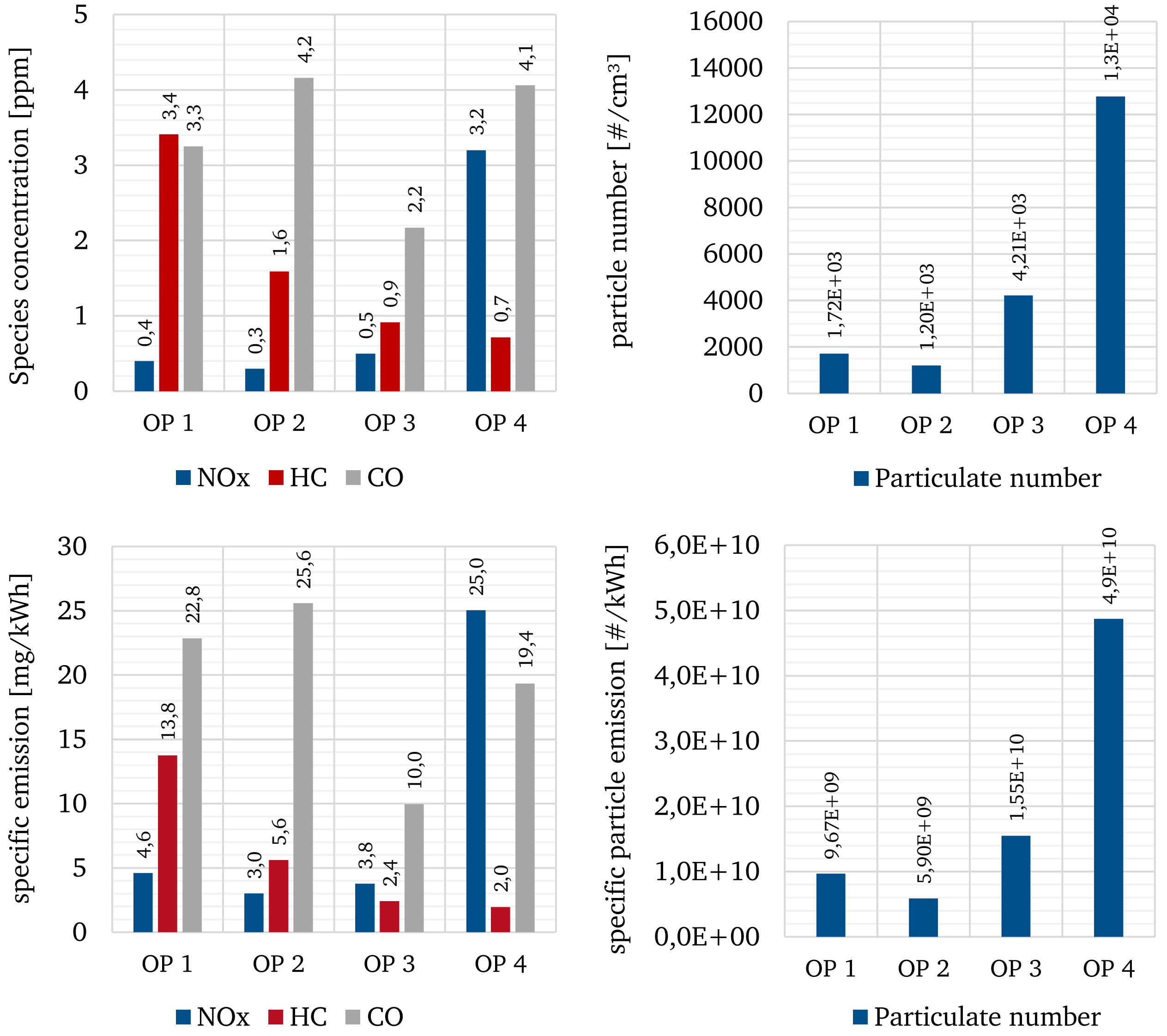

Figure 4: Emission results for regulated species of investigated operating points

Due to the over-stoichiometric operation of diesel engines, hydrocarbon (HC) and carbon monoxide (CO) emissions in general mostly exceed those of nitrogen oxides (NO_x). In the present investigation results, the intensive measures taken for NO_x conversion lead to the exact opposite effect with lower nitrogen oxides results. It should be noted that all concentration results are at or near the detection limits of the measurement equipment used. The highest NO_x concentration is measured at the highest investigated load point at a power of 33 kW with 3.2 ppm or 25 mg/kWh respectively. In order to induce the same energy in the cylinder when using OME as with diesel, almost twice as much fuel must be injected due to the lower energy content of OME. At a significantly faster combustion rate, this leads to a higher demand for heat of vaporization, which is extracted from the combustion chamber. As a result, the exhaust gas temperatures are lower with OME and since no applicative heating measures could be implemented on the engine, the EHC was used in OP 1 to heat up the exhaust gas temperature in the range above the light-off of the catalytic converters. This energy demand was considered accordingly in the specific emissions calculation. Qualitative differences between the investigated operating points that are visible in the concentration comparison remain for the power specific comparison. Within an individual operating point, the species ratio among each other changes, due to the different density of exhaust gas components. The measured particulate emissions of the raw exhaust gas are at a very low level, comparable in magnitude to those of diesel engines after particulate filter. This is a possible lever to simplify the exhaust aftertreatment system by means of reduction.

The results based on selected operating points provide a good basis for estimating the emission potentials, but are unsuitable for a classification in existing emission-immission legislation, as those are based on full driving operation. A classification must ultimately be made in driving scenarios, as this is the reference basis for the drive systems. In order to estimate the distance specific emissions during driving operation, a vehicle simulation was set up in which the combustion engine was modelled in a power split hybrid drive. For its emission behavior the previously shown results are integrated. The implemented operation strategy is used from the existing VKM toolbox. Necessary adaptations to the existing baseline version are made to ensure correct operation. However, a dedicated optimization of system components and the operation strategy parameters are not performed. As vehicle variants, the segments with the highest volume shares and their distribution on the German overall car fleet are simulated. In addition to the WLTC, the driving scenarios include various RDE routes, which are also available at VKM [10]. On the basis of the described data, a fleet average, route-specific nitrogen oxide emission of 2.3 mg/km was determined. The current limit value for diesel vehicles of 80 mg/km [11] would thus be undercut by a factor of 35. The corresponding conformity factor (CF) for this specific result adds up to CF = 0.03. This result is used as input for an immission assessment at the *Darmstadt Hügelstraße* measuring station on which the VKM immission model is based.

For the reference year of 2018 all measurement data for the calibration of the model is available. On the basis of this baseline scenario (*2018 Baseline*), estimates are now being made for changes in distance specific vehicle emissions. Since the technology in focus is based on compression-ignition vehicles, which are considered the main cause of inner-city immission exceedances, only changes to the emission factors of the diesel fleet are considered in the scenarios. The measurement scenario Darmstadt Hügelstraße is dominated by passenger cars, among which diesel vehicles account for 51.2%. Average tailpipe emissions of this year's total vehicle fleet sum up to 441 mg/km NO_x. All other parameters of the scenario remain fixed in order to be able to quantify only the influence of diesel car emissions. This applies also to the inner-city background NO_2 immission, that is kept constant at 20.9 µg/m³ and indicated by the blue bar in Figure 5. The total figure shows the immission results for the investigated scenarios.

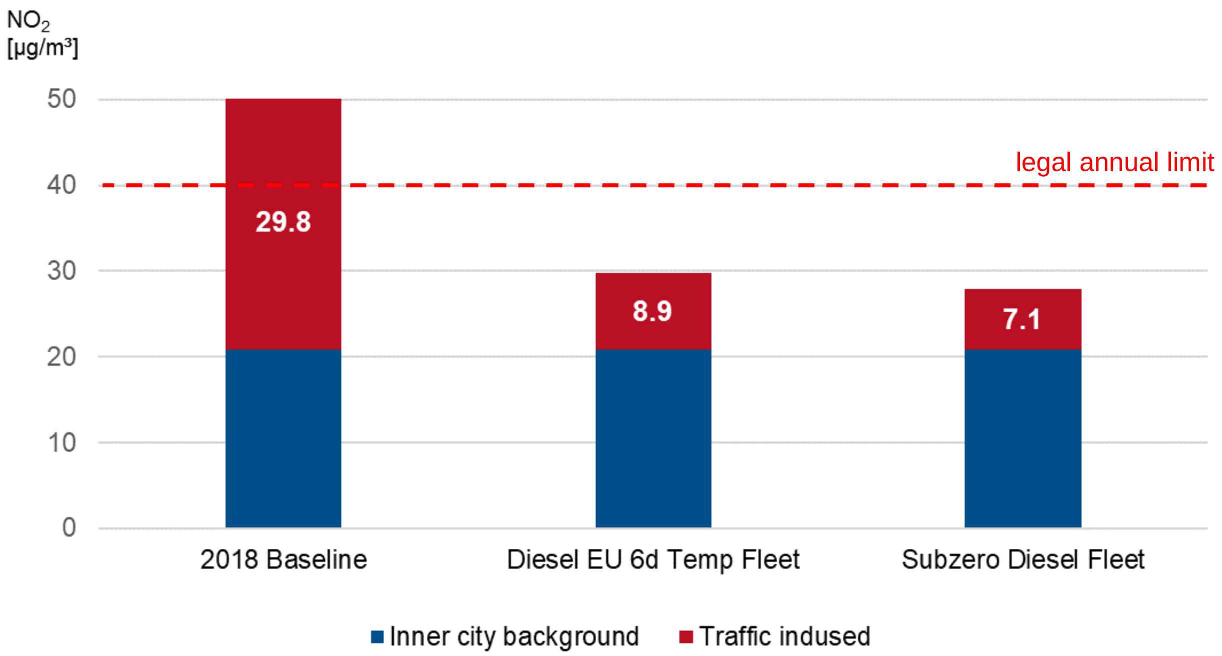

Figure 5: Calculated immission impact scenarios for Darmstadt Hügelstraße

In the first scenario, *Diesel EU 6d Temp Fleet*, all diesel passenger cars, regardless of their actual exhaust emission standard, are assumed to have the technology level EU 6d Temp. The average emission for this fleet is calculated on the basis of the publicly available RDE PEMS fleet data, that car manufacturers publish via the European Automobile Manufacturers Association (ACEA) [12]. A reduction of 20.9 µg/m³ (41%) to 8.9 µg/m³ in traffic-related immission impact compared to the 2018 baseline would be expected in the long term through natural fleet replacement, provided that the boundary conditions do not change. This means, that the annual immission limit of 40 µg/m³ would no longer be exceeded with the newest technology for passenger car (PC) diesel vehicles in the given scenario.

The second scenario, *Subzero Diesel Fleet*, the previously determined, route-specific nitrogen oxide emission of 2.3 mg/km is anticipated for all PC diesel vehicles in the simulation of the scenario. This leads to a traffic-induced additional immission of 7.1 µg/m³ and thus falls short of the result from the scenario (*Diesel EU 6d Temp Fleet*) by 1.8 µg/m³. Compared to the baseline scenario, the average tailpipe emission of the entire vehicle fleet drops from 441 mg/km NO_x to 144 mg/km (67%). With a reduction in the calculated order of magnitude, it seems obvious that the initially deferred influence of other traffic emitters is now significantly higher and has to be considered. The changing share of emitters influence is depicted in Figure 6.

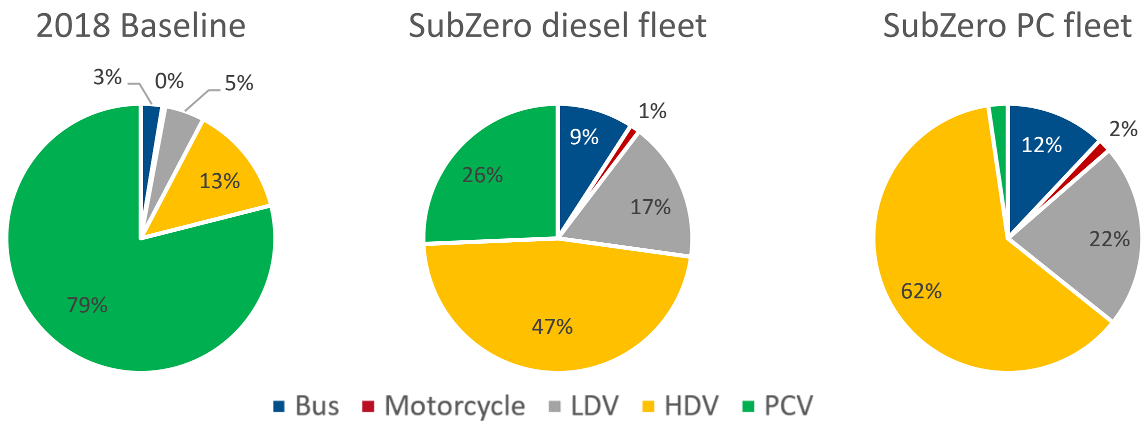

Figure 6: Share of road vehicle emitter categories in different emission scenarios

When in the *baseline* scenario 79% of the total NO_x emissions are attributable to passenger car vehicles (PCV), in the *SubZero diesel fleet* scenario this share drops to 26%, while the share of heavy-duty vehicles (HDV) increases from 13% to 47%. This phenomenon is extended in the third pie chart shown, where all PCV are substituted to SubZero emissions. In this case, the share of PCV emission is neglectable as it lies within the accuracy of the immission model, which outputs no significant immission impact anymore. With the decline of absolute PCV emissions and the other figures being kept constant, the share of other road vehicle categories increases. For further immission impact reduction these vehicle categories are the next one to be addressed.

All in all, the results indicate that the induced immission influence can be significantly reduced by the described emission scenario. The emission share of passenger cars in the SubZero scenario is reduced to a level that makes it questionable whether there is any significant contribution to the immission measurement result at all. On the contrary, with the dilution estimates given in the *Emission – Immission interaction and quantification* section of this paper, the achievable concentration level at the street side comes down to a single digit ppb concentration. Hence, the immission influence falls below the urban background in the measurement scenario. At the same time, the prevailing background concentration ranges so low that it has no influence on intake air contamination for exhaust gas cleaning. Measurements carried out at VKM show that the emission results achieved are independent of the nitrogen oxide concentration in the intake air in the area of the driving zone. To sum up, in scenarios where the immission influence of the drive system is smaller than the background immission level, an active contribution to air pollution control can be realized, since in the long term the prevailing inner-city concentration are reduced. As this is the case in the Darmstadt Hügelstraße scenario under consideration, the underlying engine, operated with OME and including its exhaust gas aftertreatment system, can be classified as a SubZero engine.

Conclusion and outlook

The present paper first introduces a definition of future vehicle emission classes within the framework of the investigations presented here. Following on from this, an immission model for nitrogen oxides developed at VKM is presented. It allows to map the immission impact for a defined measurement scenario on the basis of available data on specific vehicle emissions while considering influencing environmental conditions at the same time.

The aim of the presented investigations is to show a lowest emission potential in terms of pollutants when using a potentially CO_2 neutral fuel on a series diesel engine with currently available exhaust gas aftertreatment technology. A route-specific fleet emission potential of 2.3 mg/km is identified for nitrogen oxides under real driving conditions. In the underlying immission scenario, the reduction of the traffic-related additional pollution with a substitution of the entire diesel car fleet amounts to 76%, from 29.8 µg/m³ to 7.1 µg/m³. Diesel passenger cars would thus change from being the main cause of inner-city nitrogen oxide emissions to a neglectable influencing factor. At the same time, the impact on immissions shown is so low that the long-term use of such a vehicle fleet would lower the inner-city background level in the scenario shown. In this respect, the concept we are looking at is to be located in the SubZero area according to the introduced definition.

With regard to achievable market penetration, it should be noted that, in contrast to the pure fuel studies presented here, blends have a significantly higher potential for actual market utilization due to easier feasibility, higher availability and lower investment costs. Other studies [13][14][8] suggest that even with relatively low blending ratios, significant emission reduction potentials that would lead to the range of the presented results in this paper can be achieved.

Acknowledgement

The results presented in the paper at hand are based on a joint research project with the partners AVL List GmbH, Federal Mogul Burscheid GmbH, Schaeffler Technologies AG & Co. KG, Vitesco Technologies Emitec GmbH and Volvo Cars. The data used in the immission model was provided by HLNUG. We would like to thank for their support and good cooperation!

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