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Research Article

Possibilities of Simultaneous In-Cylinder Reduction of Soot and NO_x Emissions for Diesel Engines with Direct Injection

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Up to now, diesel engines with direct fuel injection are the propulsion systems with the highest efficiency for mobile applications. Future targets in reducing CO_2 -emissions with regard to global warming effects can be met with the help of these engines. A major disadvantage of diesel engines is the high soot and nitrogen oxide emissions which cannot be reduced completely with only engine measures today. The present paper describes two different possibilities for the simultaneous in-cylinder reduction of soot and nitrogen oxide emissions. One possibility is the optimization of the injection process with a new injection strategy the other one is the use of water diesel emulsions with the conventional injection system. The new injection strategy for this experimental part of the study overcomes the problem of increased soot emissions with pilot injection by separating the injections spatially and therefore on the one hand reduces the soot formation during the early stages of the combustion and on the other hand increases the soot oxidation later during the combustion. Another method to reduce the emissions is the introduction of water into the combustion chamber. Emulsions of water and fuel offer the potential to simultaneously reduce NO_x and soot emissions while maintaining a high-thermal efficiency. This article presents a theoretical investigation of the use of fuel-water emulsions in DI-Diesel engines. The numerical simulations are carried out with the 3D-CFD code KIVA3V. The use of different water diesel emulsions is investigated and assessed with the numerical model.

1. INTRODUCTION

Up to now diesel engines with direct fuel injection are the propulsion systems with a very high efficiency for mobile applications. Ever more stringent emission regulations, especially for particulate and NO_x emissions due to environmental and health risks, are ambitious challenges for engine manufacturers. Conventional diesel engines offer high-thermal efficiency and, therefore, will play a key role for reducing fuel consumption with regard to CO_2-induced global warming. However, the major drawbacks of these engines are the relatively high soot and NO_x emissions because of the direct fuel injection and the resulting combustion process. The combustion in conventional diesel engines leads to locally rich regions of $\lambda \ll 1$ and to local air/fuel ratios of $\lambda = 1$. This heterogeneous mixture simultaneously causes soot because of the rich areas and NO_x because of high-burning temperatures zones (Zeldovich mechanism). Utilizing conventional methods, both emission components cannot be reduced at the same time which is well known as the soot-NO_x-tradeoff [1].

Against this background, with additionally limited resources of fossil fuels, the main focus should be put on the development and use of advanced engine technologies with very low-fuel consumption and even further reduced pollutant emissions. This pressure is even more increased when taking the rapidly growing individual mobility in countries with a high-population number like China and India into account. The need to reduce CO_2 emissions and the directly related green house effect, especially in relation with the particulate matter issue of diesel engines, is due to the fact that during the last two decades dust and particulate emissions were reduced by a number of different measures and, therefore, the atmosphere is getting clearer. This results in more sunlight coming through the atmosphere which may accelerate the global warming [2]. As an important

consequence of these very complex atmospheric phenomena, the climate changing effects of fossil fuels should not be lost out of sight. Hence all measures to further reduce pollutant emissions should be put under the premise of technical solutions with optimal efficiency to achieve the lowest possible primary energy effort. Two possible ways to achieve a significant pollutant reduction already during the combustion in the cylinder are described in the following. On the one hand, an advanced injection strategy to optimize the combustion process is proposed. On the other hand, the advantages of an improved fuel by means of a diesel/water emulsion are pointed out.

2. ADVANCED COMBUSTION PROCESS

2.1. Fundamentals

A significantly contributing source for soot formation during the combustion can be the interaction of a very rich air/fuel-mixture or even liquid fuel with the flame. This effect appears especially in modern direct injection diesel engines, where the injection is often split in a pilot and a main injection due to noise reasons. After the ignition of the preinjected fuel, a part of the main injection can interact with the flame still in liquid phase or as a rich air/fuel mixture as the fuel is injected straight toward the already burning cylinder areas. This increases the formation of high amounts of soot [3].

In modern diesel engines with direct fuel injection, the injection process itself is often split in a pilot injection, a main injection, and possibly a postinjection. Usually, these part injections are done with the same injection hardware and injector and, therefore, the fuel is injected in the same cylinder areas. Hence a strong interaction between the separate part injections regarding the combustion conditions is evident.

With a small amount of fuel injected before the main injection significant reductions of combustion, noise, and NO_x emissions can be achieved compared to an engine operation without pilot injection. The preinjected fuel starts to burn before the combustion of the fuel injected during the main injection and increases the temperature in the combustion chamber. This increased temperature reduces the ignition delay for the main fuel, and the ratio of premixed to diffusion-controlled combustion is decreased. Consequently, the maximum pressure gradient and peak temperature during the combustion decrease which lowers both the engine noise and the formation of nitrogen oxides.

Unfortunately, the larger fraction of diffusion-controlled combustion leads to higher soot emissions. This becomes even more apparent with an increasing amount of preinjected fuel, where the soot emissions rise disproportionately. But, not only the larger part of diffusion-controlled combustion but also several other parameters are responsible for the higher soot emissions. The local air/fuel ratio λ for the main injected fuel is reduced due to the already burned pilot fuel, which both increases the soot formation and decreases the soot oxidation during the combustion. Additionally, a direct contact of injected and liquid fuel with the potentially still burning pilot fuel can take place and lead

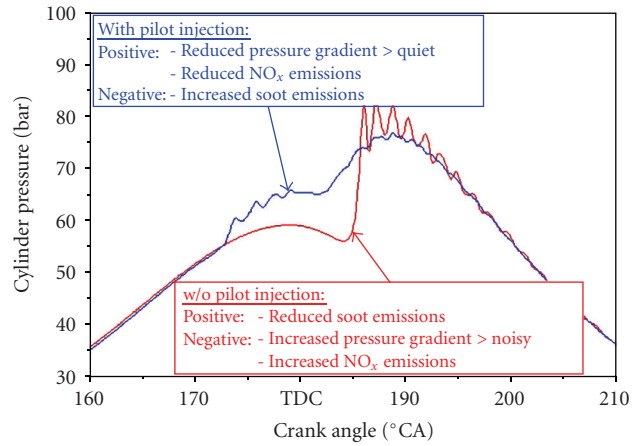


Figure 1: Cylinder pressure with and without pilot injection.

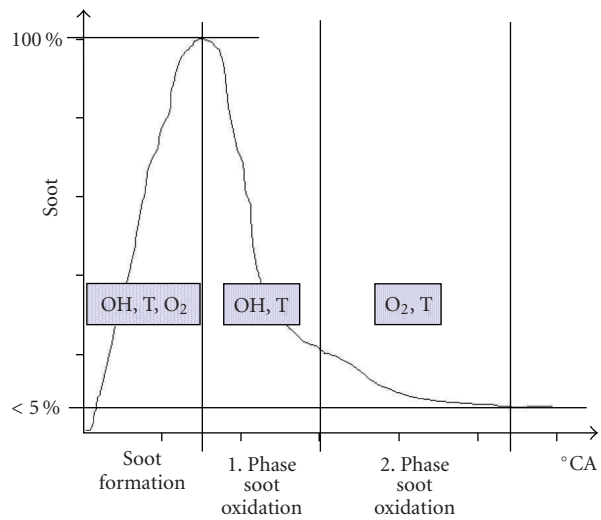


Figure 2: Qualitative characteristic process of the soot formation and oxidation [6, 7].

to an intense soot formation. Figure 1 shows an example of the cylinder pressure with and without pilot injection. The advantage of the pilot injection strategy in reducing the maximum pressure gradient due to a smaller part of premixed combustion during the combustion can be seen clearly. Nevertheless, a major disadvantage is the significantly increased soot emission [4, 5].

In Figure 2, the characteristic progression of the soot concentration in the cylinder during the combustion process is shown. This qualitative soot formation and oxidation process is found both in simulation models and different diesel and also in direct injection gasoline engines [8]. The whole process is divided into a first soot formation phase, where the in-cylinder soot concentration is rising, and afterwards two soot oxidation phases with decreasing in-cylinder soot concentration. Additionally, the corresponding main influencing parameters for the different phases are listed. It can be seen that for both the soot formation part and the second oxidation phase, the oxygen concentration

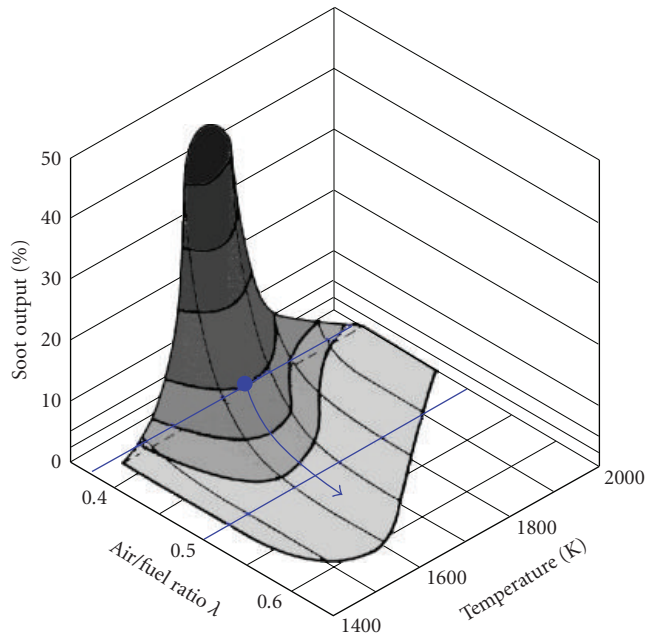


Figure 3: Temperature and λ conditions for soot formation [10, 11].

is a main parameter to influence the final engine out soot emission [9].

The effect of the local air/fuel ratio λ and the temperature on the amount of emitted soot is shown in Figure 3 [10, 11]. These results were obtained in premixed flame experiments but under pressure and temperature condition representative for diesel engines. Only a small increase in the local air/fuel ratio λ results in a significant decrease of the soot emission. Accordingly, Hansen [12] and Böhm et al. [11] also showed in extensive investigations that the soot formation could be suppressed completely when local air/fuel ratio can be kept always above $\lambda = 0.6$ to 0.7 during the combustion. Hopp [9] demonstrated in both calculations and engine experiments that the locally available oxygen content is a key parameter especially for the soot oxidation process during the combustion and hence for the engine out soot emissions.

Starting from these boundary conditions, which are influencing the soot formation, the combustion process was designed in a way to increase the locally available amount of oxygen during the combustion to lower the engine out soot emission.

2.2. Combustion process and test engine

As a reference process to evaluate the soot reduction potential of advanced heterogeneous combustion processes, the new injection strategy was chosen which is characterized by a spatial separation of the different part injections of one cycle. The spatial separation of the particular part injections as proposed should both avoid the negative interaction between pilot and main injection, in terms of fuel and flame contact, and, even more, increase the local air fuel/ratio λ for the main injection and, therefore, reduce the soot emissions as already mentioned above.

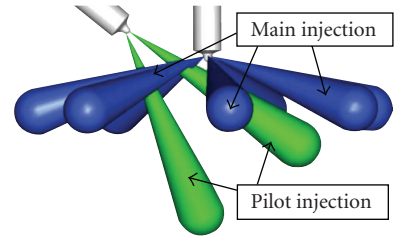


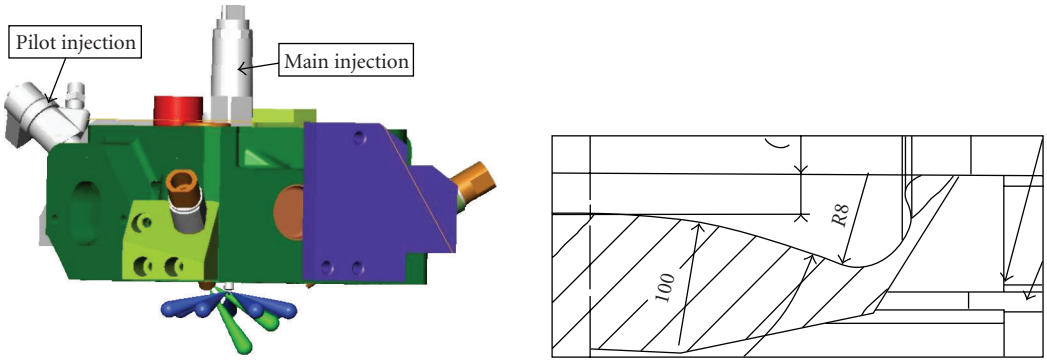
Figure 4: Schematic injection strategy.

The pilot fuel injection is directed toward the central area of the combustion chamber and later the main fuel is injected using a conventional spray pattern with a cone angle greater than 160°. With this spatial separation the fuel, injected during the pilot injection phase, burns in another cylinder area than the main fuel and hence does not reduce the local air/fuel ratio λ for the main combustion as it would be the case with a conventional pilot and main injection strategy using the same injector and spray holes.

Figure 4 shows a simple schematic drawing for the realization of the spatial separation with two pilot injection sprays and seven main injection sprays. To separate the two part injections, two different injectors were used and so the maximum possible spatial distance between the pilot and main injection is achieved.

For the investigations, a single-cylinder heavy duty research diesel engine from DaimlerChrysler was used which was significantly modified according to the experimental requirements. This engine with its four valve low-swirl cylinder head represents the current engine technology but still offers enough space to integrate the additional equipment necessary to realize the proposed injection strategy. To achieve the necessary degree of freedom concerning the injection parameters, the original unit pump injection system was replaced by a common rail system which enables the free adjustment of the rail pressure and the injection timing. The high-pressure fuel pump of the engine was also electrically driven to be able to choose the rail pressure independent from the engine operation. The second injector for the pilot injection was connected to the same high-pressure fuel rail than the main injector so the injection pressure was constant for both part injections but the timing was freely adjustable. The main injector was equipped with a seven-hole nozzle with a hole diameter of 0.2 mm and the pilot injector with a two hole nozzle with a hole diameter of 0.14 mm.

The test bench was equipped with an eddy-current brake and an electric dynamometer to either brake or crank the engine at a constant speed. Further, an external electrically driven supercharger was installed together with a water-cooled intercooler to boost the engine independent from the operating point. The engine coolant and oil was conditioned to keep the engine temperature constant at a preset value. In Table 1, the main engine specifications and operating conditions are listed.



(a) (b)

Figure 5: Cylinder head CAD-model and ω-bowl in piston.

Table 1: Engine specifications and operation conditions.

Displacement	1827 cm^3
Stroke	142 mm
Bore	128 mm
Compression ratio	17.7:1
EGR	external: 0/35%
Boost pressure	1.5 bar
Engine speed	1000 rpm
Injection pressure	1400 bar
Coolant/oil temperature	80°C

Table 2: Parameter variation.

Parameter	Values		
EGR-rate [%]	0	35	
SOE main injection [°CA]	13° BTDC to 5° ATDC		
SOE pilot injection	10° CA before SOE main		
Pilot fuel quantity [mg]	4	6	11

2.3. Cylinder head modifications

The cylinder head of the test engine was a conventional four-valve head with a centrally placed injector. This injector position was maintained for the main injection, but the production injector was replaced by a commercially available heavy duty common rail injector. For the pilot injection, a second injector was additionally integrated in the cylinder head. This injector was a production light duty injector with a specially manufactured two-hole nozzle. This smaller injector is sufficient for the pilot injection due to the significantly smaller amount of fuel for the pilot injection than for the main injection.

Figure 5 shows a CAD-model of the cylinder head with the two mentioned injectors, the schematic fuel sprays, and two additional optical accesses to the combustion chamber. Additionally, a cutout of the piston top is shown. The bowl in the piston top had a conventional ω-shape which is commonly used in direct injection diesel engine. The central area of the bowl is not very deep. This reduces the possible free spray length for the pilot fuel sprays and may lead to a nonoptimal fuel distribution for the pilot fuel injection. For the orientation of the two pilot fuel sprays, this was taken into account by not injecting directly in the middle of the combustion chamber but a little sideways.

The fuel sprays for both part injections are shown simultaneously. This is only done for a better picturing of the orientation to each other. Yet, during real engine operation the injections are temporally separated with the pilot injection toward the central area of the combustion chamber and the main injection toward the outer parts.

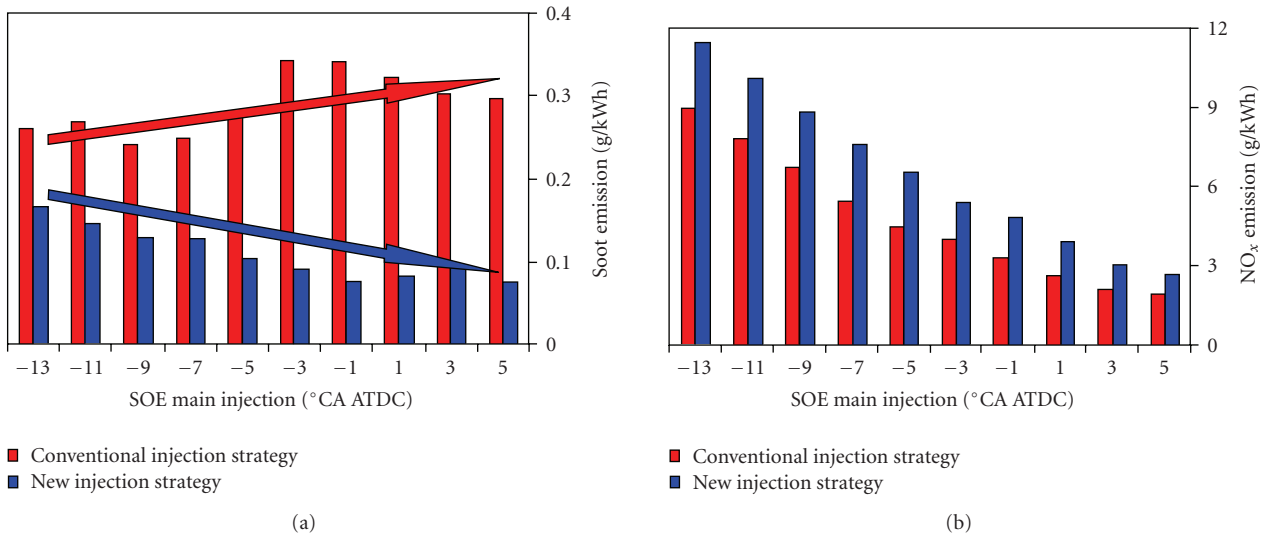
2.4. Engine operation

To assess the potential in reducing the soot emissions, the spatial separation of the pilot and main injection was compared to a conventional injection strategy where the part injections are done with the same injector. Therefore, a parameter variation concerning injection timing, fuel quantity distribution, and EGR-rate was performed when operating the engine at the same parameters but with the two different injection strategies.

In Table 2, the values for the parameter variation are listed. The engine was operated with no EGR and with 35% EGR. The injection timing was varied between 13° CA BTDC to 5° CA ATDC in 2° CA steps. In all cases, the SOE for the pilot injection was 10° CA earlier than SOE for the main injection. The fuel amounts for the two part injection were kept constant for the test with 6 mg for the pilot injection which is about 12.5% of the totally injected fuel mass. For the pilot fuel quantity variation, the pilot fuel quantity was increased while the main fuel amount was reduced to keep the total injected fuel mass constant.

2.5. Soot emissions

Figures 6 and 7 show the indicated specific soot emissions both for a conventional and a spatially separated pilot injection strategy without EGR and 35% EGR against the SOE of the main injection. As expected in both EGR cases, the soot emissions are rising with later injection



(a) (b)

Figure 6: Soot and NO_x emissions with injection timing variation and 0% EGR.

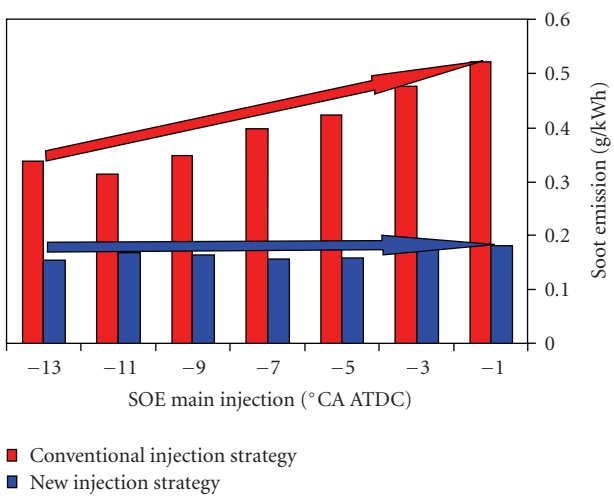


Figure 7: Soot emissions with injection timing variation and 35% EGR.

timing when using a conventional injection. For the new injection strategy and no EGR, the soot emissions are slightly decreasing with later injection which was actually not expected. A possible explanation for this behavior could be worse mixture formation condition for the pilot fuel spray in terms of poor combustion chamber geometry with a lower piston position for earlier injection timings. The two pilot fuel sprays may reach the edge of the piston bowl and subsequently increase the soot formation. With an EGR-rate of 35%, the soot emissions remain almost on a constant level independent of the injection timing. Both a longer ignition delay and a better evaporation caused by the recirculated exhaust gas may improve the mixture formation and avoid an increase of the soot formation with earlier injection timings.

These results approve the assumed influence of the local air/fuel ratio λ on the soot formation and oxidation process. Only a minor increase of the local λ by separating the pilot fuel burning areas spatially from the main fuel burning areas reduces the soot emissions significantly as expected according to the soot formation theory [10, 12].

2.6. Combined soot and NO_x reduction potential

To identify the full potential of the combustion process with the spatially separated pilot and main injection strategy, the emission behavior of the engine regarding both the soot and NO_x emissions in combination has to be taken into account. Figure 8 shows the soot and NO_x reduction potential for an SOE of the main injection at 1° CA BTDC. This injection timing still allows an engine operation with a high-thermal efficiency. Starting point for the emission comparison, defined as 100%, is an engine operation with a conventional pilot injection strategy and 0% EGR. If the EGR-rate is increased to 35% for the conventional injection, the common soot-NO_x-tradeoff is still present and the soot emissions rise to 160%, while the NO_x emissions go down to 30% (q. v. Figure 8 upper diagram). Comparing the same starting point of the conventional injection with the new injection strategy and 35% EGR both the soot and NO_x emissions are roughly halved (q. v. Figure 8 lower diagram). The reason for this simultaneous reduction is the high soot reduction potential of the new injection strategy which allows an engine operation with higher EGR-rates to achieve significant NO_x reductions without having the drawback of severely increased soot emissions. Incidentally, even a further reduction of the soot emissions would be possible if the EGR-rate would not be increased that far as can be seen in Figure 6 (upper diagram) for the no EGR case. Without adding EGR soot, emission reductions of up to 80%, compared to the conventional split injection, are possible. A 20 to 40% increase of the NO_x emission has to be accepted then as can be seen in Figure 6 (lower diagram).

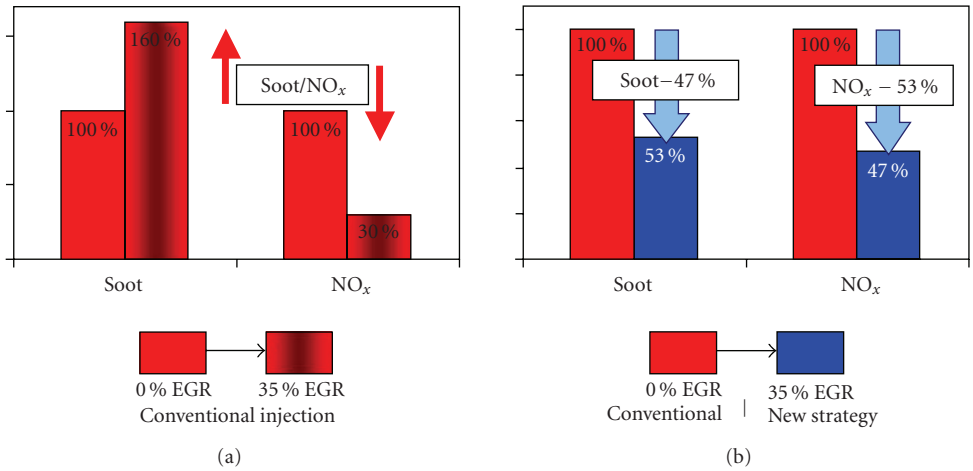


Figure 8: Potential for simultaneous soot and NO_x reduction.

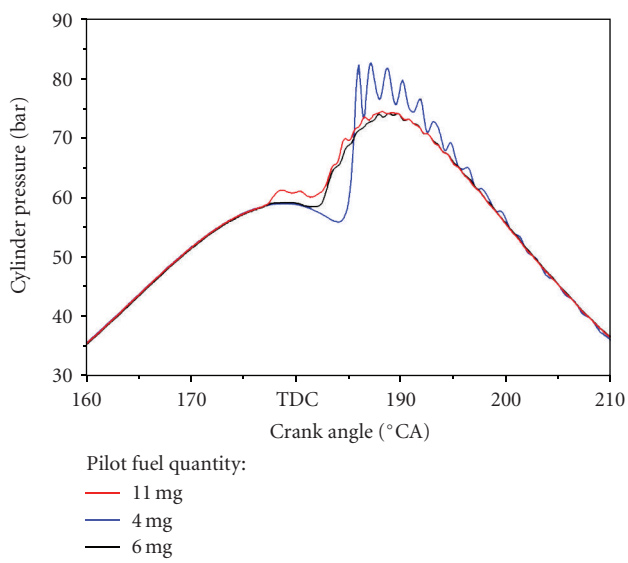


Figure 9: Cylinder pressure with conventional pilot injection.

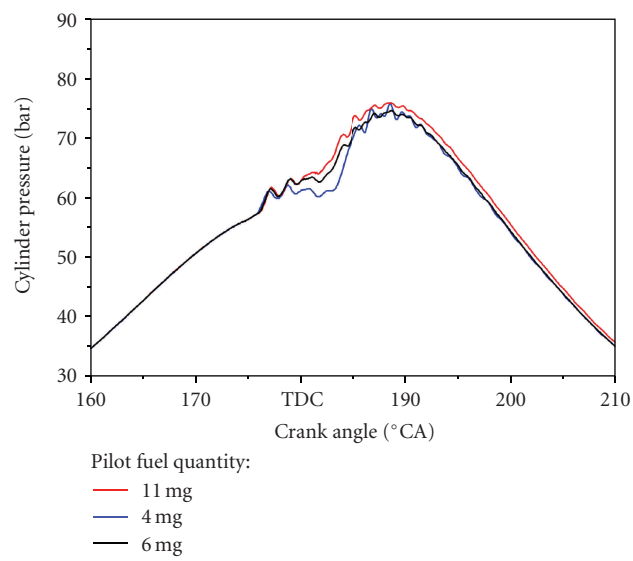


Figure 10: Cylinder pressure with spatial separation of pilot and main injection.

Generally speaking, the obtained results have shown that advanced heterogeneous combustion processes still offer a significant potential to reduce the soot and NO_x emissions simultaneously. When applying EGR, this NO_x reduction can be achieved without any negative effects on the combustion efficiency compared to a conventional pilot injection strategy. Concerning the HC and CO emissions, the experiments have shown that there is virtually no difference between conventional and new pilot injection strategy and they are, as expected for heterogeneous diesel combustion, on a low absolute level.

2.7. Combustion behavior for different pilot fuel quantities

Figures 9 and 10 show the cylinder pressure traces for the conventional and the new pilot injection with 4, 6, and 11 mg fuel for the pilot injection. For the conventional pilot injection, a significant difference in the cylinder pressure traces can be seen. For the smallest amount of pilot fuel of 4 mg, no effect on the combustion could be observed and the combustion process is similar to a single main injection. With a fuel quantity of 6 mg, only a very small pilot combustion in the cylinder pressure can be seen, but this is sufficient to reduce the ignition delay, the premixed combustion part, and hence the maximum pressure rise significantly. For the 11 mg pilot fuel amount almost no difference in the main combustion, but a further increased pilot combustion is evident. The shift in the combustion timing for the main injection and the ignition delay of the main injection changes reduces the ratio of premixed to diffusion-controlled combustion and hence, in combination

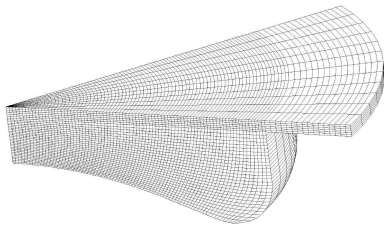


Figure 11: Computational grid of the heavy duty DI diesel engine.

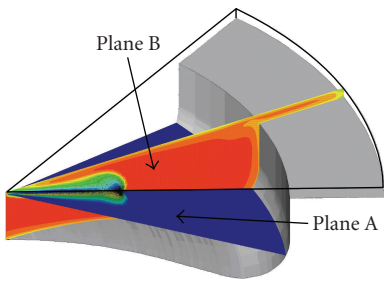


Figure 12: Computational grid of the heavy duty DI diesel engine.

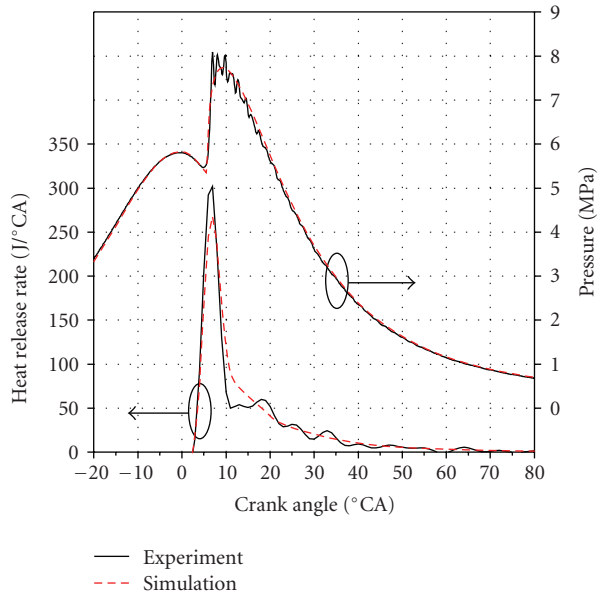


Figure 13: Computational grid of the heavy duty DI diesel engine.

with the already described λ-effect, increases the soot emissions.

This looks completely different for the spatially separated pilot injection as shown in Figure 10. In contrast to the conventional injection also for the smallest amount of 4 mg fuel a pilot combustion and its effect on the main combustion in reducing the maximum pressure gradient can be seen in the cylinder pressure. By increasing the pilot fuel quantity, there is almost no shift in combustion timing, only the amount of released heat for the pilot combustion is certainly higher. Because of the constant combustion timing and ignition delay for the main injection, the ratio of premixed to diffusion-controlled combustion stays constant resulting in almost constant soot emissions.

Additionally, the spatial separation of the fuel injection has two further advantages.

First, an increasing amount of pilot fuel is not reducing the initial local air/fuel ratio λ for the main injection. In fact with a higher amount of pilot fuel the combustion conditions for the main injection concerning the available oxygen are even improved as less main fuel is then injected for the same load conditions.

Second, as the pilot fuel is not injected through the same nozzle holes as the main injection the nozzle layout can be optimized for the much smaller amount of pilot fuel. For example, only two holes are used for the pilot injection instead of using the seven holes of the main injector. This also improves the mixture formation for the spatially separated pilot injection compared to the conventional pilot injection.

Summarizing the pilot fuel quantity variation results, it can be stated that the spatially separated pilot injection has a significantly higher pilot quantity tolerance concerning the soot formation and therefore the complexity of the small fuel amount control can be reduced.

Table 3: Injection parameters for the base case.

	Diesel ($y_{0,\text{Diesel}} = 1.0$)	Emulsion ($y_{0,\text{Diesel}} = 0.75$)
Nozzle	A	A
p_{inj} [MPa]	140	140
m_{inj} [mg]	120	160
SOI [°ATDC]	−4	−4
DOI [°]	17.54	22.40

3. FUEL/WATER EMULSION

3.1. Fundamentals

Another promising method to reduce emissions of nitrogen oxides and particulates in direct injection diesel engines is water introduction into the combustion chamber. Various introduction strategies with their particular advantages and disadvantages with respect to emissions and applicability in different engine applications are possible. For obtaining maximum improvements, water has to be added at the right spot at the right time [14]. In conventional, heterogeneous diesel combustion, nitrogen oxides are mainly formed by the highly temperature-dependent Zeldovich mechanism. All water introduction strategies aim at reducing the temperatures in the combustion chamber. The effect of water introduction is two-fold: water reduces the temperature by its large enthalpy of vaporization and the larger heat capacity compared to dry air.

Injection of emulsions places the water at the right spot in the spray region. As a result, NO_x emissions can be reduced significantly. Furthermore, emulsions offer the potential to also reduce particulate emissions, for example [14–17]. However, some authors also report a neutral or even negative effect of emulsions on particulates, at least

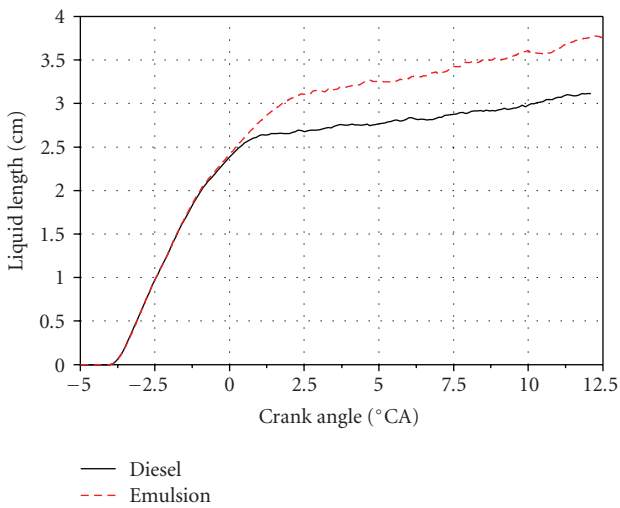


Figure 14: Liquid penetration under nonreacting conditions.

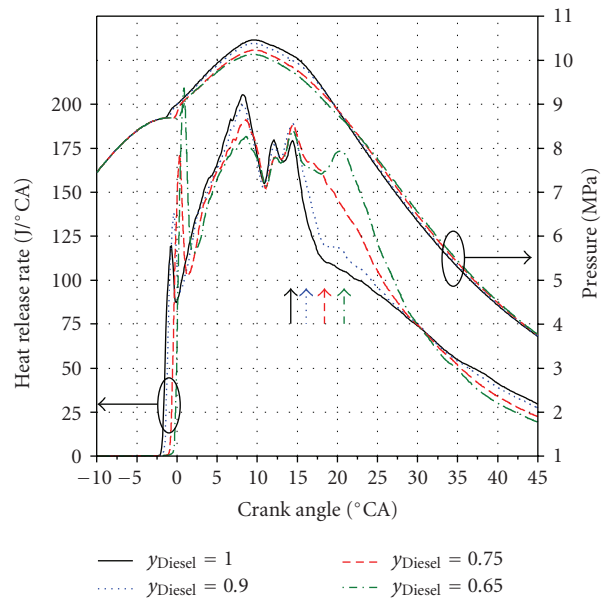


Figure 16: Heat release rate and pressure history for fuels with different water contents.

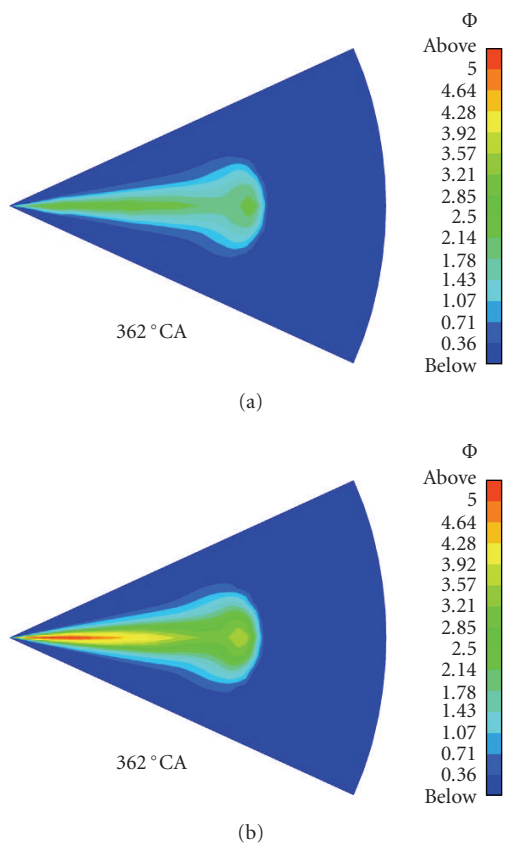


Figure 15: Equivalence ratio in the emulsion spray (upper) and diesel spray (lower), cutplane A.

in some points of operation (e.g., [17, 18]). For example, Matheaus et al. [17] found drastically increased values of particulate matter, unburned hydrocarbons, and CO at idle operation in a heavy duty diesel engine. Musculus et al. [19] attributed this to a possible cylinder wall wetting at this point of operation due to the increased liquid penetration of diesel fuel-water emulsion compared to pure diesel fuel.

There are different chemical and physical mechanisms that possibly explain a reduction of soot emissions. One possible mechanism is the occurrence of the so-called microexplosions of emulsified fuel droplets that lead to a better atomization and thus air-fuel mixing [20]. This violent rupture of droplets has been observed in numerous single droplet evaporation experiments, for example [21]. While some investigations on sprays have been conducted, there does not seem to be clear evidence that microexplosions occur in modern DI diesel engine combustion process.

In principle, the use of diesel fuel-water emulsions is possible without any major modification of the injection equipment. Of course, since the emulsion has a lower heating value than pure diesel fuel, the injection system has to be modified in order to keep the rated engine power constant. A drawback of emulsified fuels is the longer ignition delay and problems associated with cold-start and idling operation.

The various water introduction strategies offer a high potential in improving diesel engine emissions. Thus it is necessary to gain a better understanding of the different processes involved during combustion with these techniques and develop numerical models able to capture these effects. This section of the paper presents a first step toward developing these capabilities in multidimensional combustion modeling and focuses on diesel fuel-water emulsions. The computational model has been already validated on single droplet evaporation experiments [22]. Here, the model was used to investigate diesel fuel-water emulsion combustion in a heavy duty diesel engine.

The 3D-CFD code KIVA-3V [23] was used for the calculations in this study. The code solves the mass, momentum, and energy conservation equations coupled with the RNG

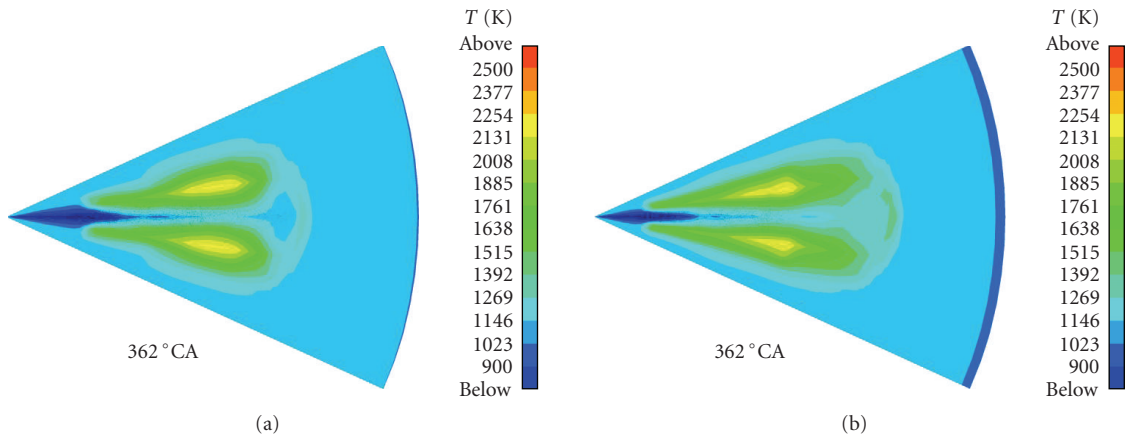


Figure 17: (a) Temperature distribution of the 25% emulsion; and (b) pure diesel fuel flame, cutplane A.

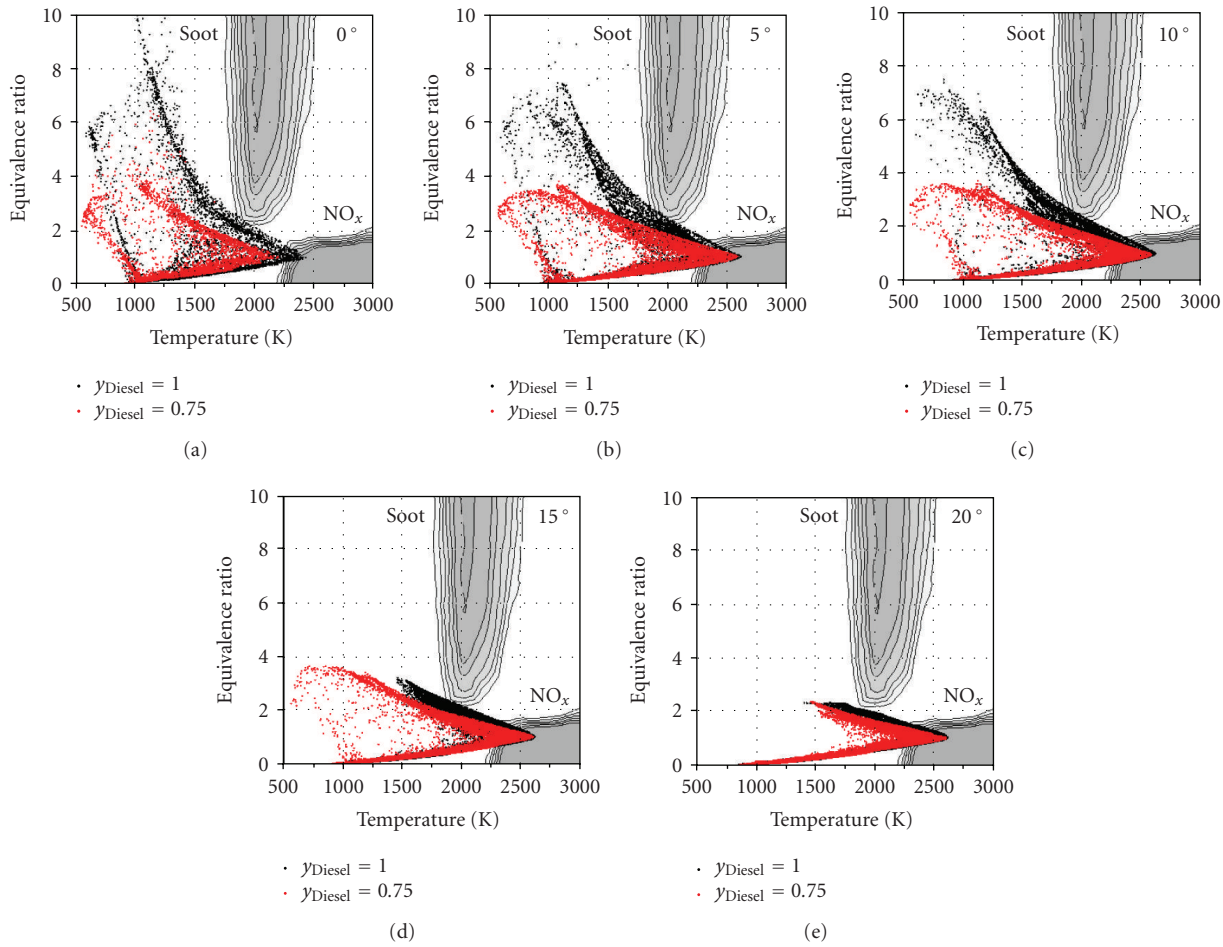


Figure 18: Equivalence ratio-temperature plots for pure diesel fuel and a 25% emulsion; Soot and NO_x formation maps according to [13].

k-ε turbulence model in three dimensions as a function of time. Various differences to the original code in the physical and chemical submodels describing the interactions between spray droplets and the gas phase, ignition and combustion were employed in this study. For example, the primary breakup of droplets was modeled by the Blob-model and the secondary breakup by the Rayleigh-Taylor and Kelvin-Helmholtz hybrid model, the droplet evaporation by using a semicontinuous evaporation model, ignition by the Shell ignition model and the emission formation for

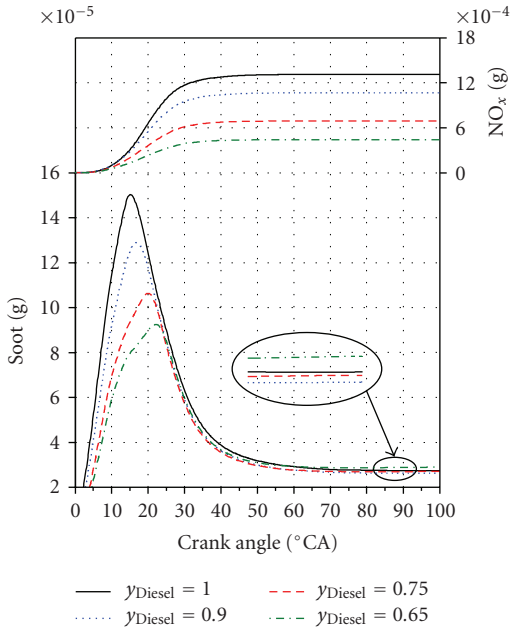


Figure 19: Soot and NO_x history for different fuels.

nitrogen oxides by the extended Zeldovich mechanism, soot formation by the Hiroyasu model, and its oxidation by the Nagle and Strickland-Constable model. For further details of the different models used for the calculation please refer to [22].

3.2. Numerical results

The engine considered here was a heavy duty DI diesel engine with a bore of 128 mm, a stroke of 142 mm, and a compression ratio of 17.7:1. The engine was retrofitted with a common-rail fuel injection system and utilizes a low swirl-combustion process. A seven-hole nozzle in a centrally located injector was used.

When using the same injection equipment with emulsified fuels, it might not be possible anymore to obtain maximum power because the injection durations become too long. Thus in addition to the base nozzle, a modified nozzle was used in some of the calculations. The modified nozzle has been adjusted in order to obtain the same injection durations for an emulsion with 25% water content compared to the original nozzle with pure diesel fuel when injecting the same fuel energy. For this modification, it was assumed that both nozzles have the same discharge coefficient. The original nozzle (nozzle A) had a hole diameter of 200 μm, the modified nozzle (nozzle B) a diameter of 225 μm.

For the simulations, only 1/7 of the combustion chamber was modeled, taking advantage of the axissymmetric nature of the problem. The calculations were only performed between IVC and EVO. Figure 11 shows the computational grid that was used for the heavy duty engine. The grid consisted of approximately 110500 cells at BDC and 33800 cells at TDC. Figure 12 shows the location of cutplanes used in subsequent figures.

Figure 13 exemplarily shows a comparison between experimental and numerical results for a lower part-load point of operation. Here, the heat release rate was computed for both the experiment and the simulation by a pressure analysis software. For all other cases, the heat release rate was taken directly from the simulation. There is a good agreement for both pressure and heat release rate.

All of the following calculations were performed at a single point of operation at upper part load and an engine speed of 1750 min^{-1}. Except where otherwise stated, an emulsion with a water content of 25% by mass was used. For all calculations, the injected mass was adjusted in order to maintain the same indicated mean effective pressure of the calculated part of the high-pressure cycle. For larger fuel masses, the injection pressure was kept constant and the injection duration was prolonged. Table 3 shows the injection parameters for the base case.

3.3. Nonreacting conditions

To compare the behavior of pure diesel and the emulsion, a first set of calculations was performed to investigate the spray behavior under nonreacting conditions.

The liquid spray length for both fuels is shown in Figure 14. Until the penetration of diesel reaches a plateau, the penetration of both fuels is nearly identical. For the emulsion, the steady liquid penetration length is reached later than for diesel fuel. This is in correspondence with the slower evaporation of emulsified fuel droplets. While the longer liquid penetration is uncritical under the given conditions, the emulsified fuel will have a higher risk of fuel impingement on the piston walls at low load or idle operation.

Figure 15 visualizes the equivalence ratio in cutplane A for the two fuels at 2° ATDC. Here, the equivalence ratio was defined as the ratio of oxygen atoms necessary to oxidize all available carbon and hydrogen atoms and the actually available amount of oxygen atoms. Since water displaces a certain amount of diesel fuel, the mixture in the emulsion spray is significantly leaner. Especially, the very high value of $\Phi \approx 5.0$ near the nozzle when using pure diesel is reduced to $\Phi \approx 3.0$ for the emulsion. The reduced equivalence ratio will have an important impact on soot formation chemistry.

An analysis was carried out to estimate the kinetic limit of superheat of fuel water emulsion droplets. Some of the droplets in the spray exceed this limit. However, all these droplets are extremely small (below 1 μm) and it is thus not likely that these droplets would microexplode or that these microexplosions would have a dramatic effect on the spray. However, the current analysis is not adequate to fully assess the occurrence and influence of microexplosion.

3.4. Reacting conditions

Figure 16 compares the pressure history and heat release rate for fuels with different water contents. The start of injection was held constant at −4° ATDC. The ignition delay and thus also the premixed burn fraction continuously increases with increasing water content of the fuel. The end of injection

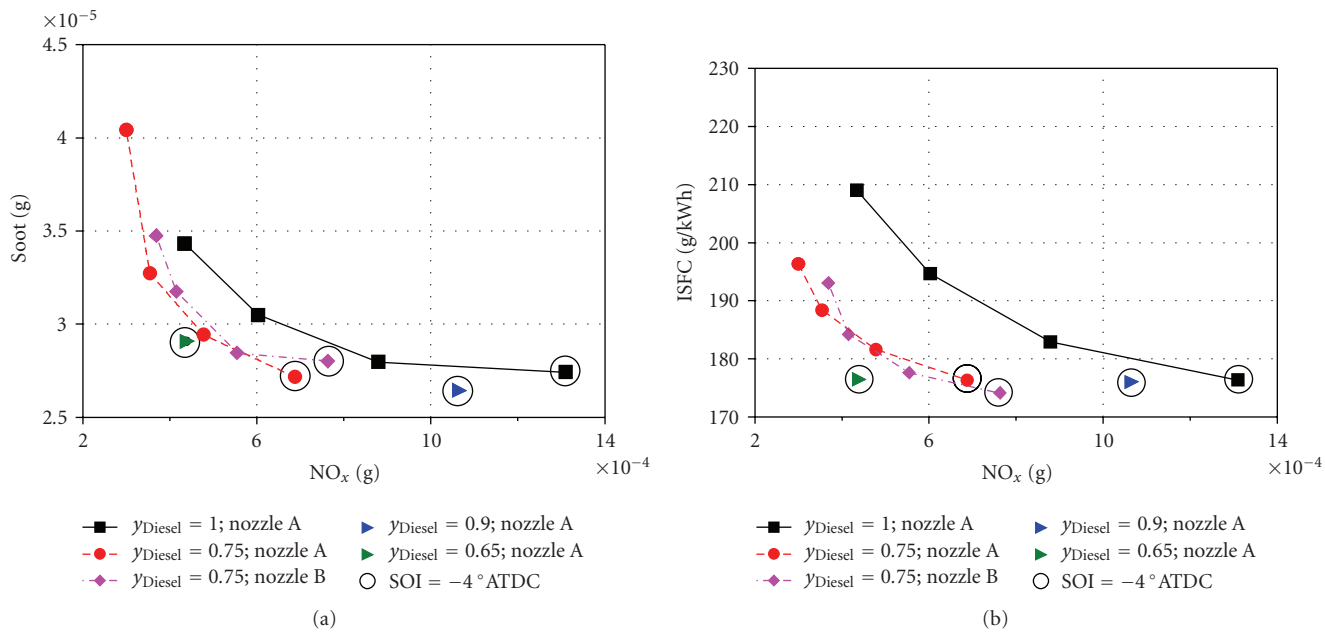


Figure 20: Soot-NO_x and ISFC-NO_x tradeoff.

of the different cases is indicated by arrows in Figure 16. Because of the longer injection duration, the point where the heat release rate drops is shifted to later times for higher water fractions. As a result, the MFB50 point is shifted only slightly to later times and differs by approx. 1° for pure Diesel and the 35% Emulsion. Figure 17 exemplarily shows the temperature distribution in cutplane A for the 25% emulsion and pure Diesel fuel at 2° ATDC. As can be seen, the lift-off distance of the diffusion flame is increased for the emulsion. Flame lift-off is an important characteristic of a Diesel engine combustion process [24]. An increased lift-off length reduces the equivalence ratio in the diffusion flame, because the amount of entrained air increases with distance to the nozzle. This reduction in the equivalence ratio is in addition to the reduction already shown in the preceding section.

The improved equivalence ratio in terms of soot formation is shown in Figure 18. The idea of Akihama et al. [13] is followed, plotting the equivalence ratio over temperature for all individual computational cells. Also shown are the regions of soot and NO_x formation, which were also adopted from [13]. Note that the location of these regions depend also on other thermodynamic parameters and the type of fuel and are given only as a guideline. At TDC there is significant scatter for both fuels because the diffusion flame is not fully established. At later times, the typical shape of a diffusion flame is obtained with the highest temperatures in the slightly rich region. It can be seen that the equivalence ratio in the cells of the emulsion flame are shifted away from the soot formation region compared to Diesel fuel. While not as significantly, the thermodynamic states, where high NO_x formation occurs are also reduced. Since NO_x formation is extremely dependent on peak temperatures, already a small reduction in peak temperature will lead to a large reduction in nitrogen oxide emissions.

Figure 19 shows the predicted nitrogen oxide and soot history. As expected, the formation of NO_x is drastically reduced with increasing water content. While the peak soot mass is continuously reduced with higher water concentrations, the soot mass at EVO has a minimum for the emulsion with 10% water fractions and increases again for higher water fractions. While a very simple soot model was used here, the occurrence of such a minimum seems reasonable, since there will be a tradeoff between the reduction in soot formation due to the lower equivalence ratios and a reduction of soot oxidation due to the lower combustion temperatures. However, the oxidation of soot by OH-radicals was neglected in the current soot model and the increased OH-radical concentration with increasing water content might have an important influence on soot oxidation.

Finally, Figure 20 shows the soot-NO_x and the ISFC-NO_x tradeoff for a variation of the start of injection under constant load. Since the specific fuel consumption ISFC has been calculated with the IMEP which was in turn calculated from IVC to EVO, the fuel consumption values can only be seen in qualitative terms. In addition to the trends of pure diesel fuel and the emulsion with 25% water content using nozzle A, results are also shown for the 25% emulsion with nozzle B. There is a clear advantage in the tradeoff for the emulsified fuel with both nozzles. Comparing the optimal point in terms of emissions, the reduction in nitrogen oxides with the 25% emulsion is approximately 21%. This is in accordance with a "rule of thumb," predicting a reduction of 10% in nitrogen oxides for 10% of water addition [14, 18]. Specific fuel consumption is also improved when using the emulsified fuel. This numerical result is in contrast to some

results from the literature [14], while in accordance with other [16]. The influence of the emulsification on ISFC will depend strongly on the kind of engine operation and the specific injection system used in the investigations.

In future studies, a validation with engine test data will extend the verification of the computational model performed in this study. Furthermore, a phenomenological soot model that better captures physical effects will be used in the future. This includes the effort to capture the important effect of an increased OH-radical concentration due to the addition of water on the soot oxidation.

4. SUMMARY

Two different measures to improve the soot-NO_x and the ISFC-NO_x tradeoffs. The first concept uses an advanced heterogeneous CI combustion processes which still offer substantial possibilities to reduce the critical soot and NO_x emissions while maintaining a high-thermal efficiency. Due to comfort and NO_x reduction reasons modern diesel engines with common-rail injection systems usually use a small pilot injection before the main injection which effect is mainly a shorter ignition delay for the main combustion. But this can lead to increased soot emissions. The combustion process discussed in this paper with a spatial separation of the pilot from the main injection represents an advanced CIDI process which avoids the negative effect of the pilot injection on the soot formation while still maintaining its positive effects on NO_x and noise. The results have shown that besides reduced soot emissions also substantially reduced NO_x emission can be achieved due to the improved EGR-tolerance of the combustion process without increasing soot.

Furthermore, the potential of using diesel fuel-water emulsions in the diesel combustion process has been investigated numerically. Here, also improved soot-NO_x and ISFC-NO_x tradeoffs were predicted with the CFD-calculations. First, experimental results confirm these predictions and allow a further optimization of the relevant calculation models.

NOMENCLATURES

y_{Diesel}: Mass fraction of diesel in emulsion
Φ: Equivalence ratio
ATDC: After top dead center
BTDC: Before top dead center
CIDI: Compression ignition direct injection
DOI: Duration of injection
EGR: Exhaust gas recirculation
IMEP: Indicated mean effective pressure
ISFC: Indicated specific fuel consumption
MFB50: 50% of fuel mass burned
NO_x: Nitrogen oxides
SOE: Start of energizing
SOI: Start of injection
TOE: Time of energizing.

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