Studying Equivalence ratio – Temperature Maps in a Heavy-Duty Diesel Engine

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Abstract
New measurements have been done in order to obtain information concerning the effect of EGR and a paraffinic hydro-treated fuel for the smoke and NOx emissions of a heavy-duty diesel engine. The measured smoke number and NOx emissions are explained using detailed chemical kinetic calculations and CFD simulations. The local conditions in the research engine are analyzed by creating equivalence ratio – temperature (Phi-T) maps and analyzing the CFD results within these maps. The study uses different amount of EGR, Miller cycle, and two different diesel fuels; standard EN590 diesel fuel and a paraffinic hydrotreated vegetable oil (HVO). The detailed chemical kinetic calculations take into account the different EGR rates and the properties of the fuels. It was observed that NOx emission trends can be well captured with the Phi-T maps but the situation is more difficult with the engine smoke.

Keywords: Phi-T maps, combustion simulation, diesel engine, emissions

1. Introduction
Phi-T maps were first introduced by Kamimoto and Bae [1]. Afterwards Phi-T maps have mainly been used in theoretical studies to identify beneficial trajectories [2], clarify soot formation paths [3] and to understand the local conditions in the engine combustion chamber [4]. Phi-T maps are useful tools but they lack some exactness as pointed out by Bergman et al. [4]. This is because the Phi-T maps do not take into account mixing between different parts of the map. In addition, as observed by Pickett et al. [3], the path that leads to soot formation matters; not only the end state of combustion. Nevertheless, Phi-T maps can be used to study the local combustion conditions in the combustion chamber.
In this study experimental data is utilized to explain how Phi-T maps can be interpreted. New measurements have been carried out in order to obtain information concerning the effect of EGR and a paraffinic hydro-treated fuel for the smoke and NO$_x$ emissions of a heavy-duty diesel engine. The bio-derived hydrotreated vegetable oil (HVO) used in the study is available as a commercial product under the name NexBTL from the Finnish oil company Neste Oil. The HVO oil contains mainly parafinic compounds and it has no aromatic components, and it also has very high cetane number (>90). Using the HVO fuel, the smoke emissions are lower than with standard EN590 diesel fuel. NO$_x$ emissions are also lower due to high cetane number (low ignition delay) and lower density (longer injection duration).

The Phi-T maps have been constructed using detailed chemical kinetics and taking the EGR rate into account. CFD results have been plotted onto the maps and the observed trends from the Phi-T maps have been compared with the experimental results. Furthermore, Miller cycle has been compared to the above mentioned EGR addition. The idea of Miller cycle is to lower the charge air temperature before combustion. With the lower gas temperature a decrease in NO$_x$ emissions is aimed at. The lower top dead center (tdc) temperature is typically achieved by changing the valve timing in the engine. The utilization of the Miller cycle may sometimes cause increased soot emissions. The combination of detailed kinetic calculations, the new measured data, and the CFD analysis is found valuable in analyzing the Phi-T maps together with the measured engine emissions. This paper suggests that rather accurate NO$_x$ trend predictions can be made by using Phi-T maps. On the other hand, the accuracy of sooting behavior seems to be on a more vague state.

### 2. Experimental Engine

The single-cylinder research engine is based on a commercial 6-cylinder off road common rail diesel engine. Cylinder dimensions are standard from the production engine, see Table 1.

The research configuration consists of the engine and an electrical motor for braking and motoring the engine. The control and measurement system is made in house at Aalto University. The engine has a very flexible control system. It has a completely independent charge air system equipped with an independent EGR system using pure nitrogen. The control system allows full control over rpm, charge air pressure and temperature, exhaust back pressure, EGR percentage, injection timing, injection pressure, and injection duration. Also multiple injections per cycle are possible. The engine is equipped with common rail fuel injection system.

In addition, the engine has been equipped with hydraulic valve actuators in order to have full freedom of the opening and closing times of the valves as well as the opening duration and magnitude of the valves.

Smoke emissions have been measured by Fuel Smoke Number (FSN) meter by AVL 415S. This method uses a filter in the exhaust pipe. The darkness of the filter color is measured optically after each measurement point. NO$_x$ is measured with Ecophysics CLD 822Sh.
The mechanism to describe the PAH formation and destruction is based on a mechanism developed by Naydenova [5]. In this mechanism the C1-C4 hydrocarbon oxidation mechanism originates from Hegesh [6], the C2 mechanism from Wang and M. Frenklach [7]. Reactions for C3-, C5- to C8-hydrocarbons are based on the work of Richer and Howard [8], Skjoth-Rasmusseen et al. [9] and Frenklach and Warnatz [10]. The n-heptane model was adopted from Correa et al. [11] The formation and growth of polycyclic aromatic hydrocarbons is based on the HACA model [12], Additional reaction paths of PAH formation and growth for PAH between benzene and pyrene were adopted from Richter et al. [13], together with several reaction paths for large polycyclic aromatics up to coronene. In this work, the mechanism of Naydenova [5] was extended with a set of reaction describing nitrogen chemistry from Coda Zabetta et al.[14] The complete mechanism contains 238 species and 1505 reactions. The subset describing the nitrogen chemistry consists of 194 reactions.

4. CFD Model

The engine was modeled with a sector mesh that represents one fuel spray in the engine. The mesh at tdc is shown in the Figure 1. The k-ε RNG turbulence model is used. The Reitz-Diwakar drop breakup model [15] is used together with the O’Rourke droplet collision model [16] with some improvements and additions as discussed in [17]. The mass transfer from the droplets due to evaporation is modeled according to Bird et al. [18]. The mass transfer coefficient is modeled according to Ranz and Marshall [19]. The initial half spray opening angle was set to a constant value of 10 degrees.

The fuel injection profile obtained from 1-D simulations [20]. The mass flow rate of injected fuel has been simulated with GT-Fuel. The model consists of rail and high pressure pipe and an injector. A rail pressure of 450bar was used in the study. Discharge coefficient of the nozzle holes was calculated using combined Giffen-Muraszew and Schmitt model, in Figure 2. The obtained mass flow rate is also shown in the Figure 2. This mass flow rate curve was used as a boundary condition in the fuel injection CFD modeling.

The combustion model used is ecfm-3z that is described e.g. in [21]. The model divides the reactions between premixed and mixing controlled combustion, and between non-reacting and reacting parts. The premixed combustion is computed from flame surface density equation. The reaction rate in the mixing controlled phase is related to the turbulent characteristic time. Three-step main chemistry is used with this model.
Figure 1 - Computational sector mesh (1/8 of the total cylinder) in the CFD simulations at top dead center position. The mesh has 12760 cells at tdc position.

Figure 2 - Combined Giffen-Muraszew and Schmitt –model for flow coefficient of nozzle hole (left). Fuel injection profile used in the CFD simulations obtained from 1-D simulations (right). The engine load is 50% and the maximum injection pressure is 450bar.

Mixture fraction is frequently used in combustion models used in CFD. The mixture fraction is a conserved scalar that describes the mass fraction of the mixture that originates from the fuel. When the stoichiometric mixture fraction is known, lambda and equivalence ration can be calculated from the stoichiometric mixture fraction and the local mixture fraction. Using this approach lambda represents the lambda of the fresh mixture and will not change as the combustion process proceeds.

Miller cycle is simulated so that the tdc average temperature is 97K lower than in the normal cycle (952K vs 855K). The charge air mass was increased by about 10% and bottom dead center pressure was decreased 0.067bar in the Miller cycle simulation compared to the standard cycle. In experiments, this is achieved by closing the intake valve earlier than in the standard cycle. This results in gas expansion that lowers the gas temperature. At the moment, no directly comparable Miller cycle experiment is available.

5. Results

5.1 Smoke number (FSN) and NO\textsubscript{x} emissions

Figure 3 shows the measured fuel smoke number (FSN) and NO\textsubscript{x} emissions. The figure shows that EGR strongly reduces NO\textsubscript{x} emissions but also increases smoke. Using the paraffinic HVO fuel seems to suppress the smoke production. It also has positive influence to the NO\textsubscript{x} emissions.
The EGR rate is defined in the experiments and in the simulations as

\[
\text{EGR} \, \% = \frac{\dot{m}_{N_2,\text{EGR}}}{\dot{m}_{\text{Tot}}} \times 100
\]  

(1)

where \( \dot{m}_{N_2,\text{EGR}} \) is the EGR nitrogen mass flow rate and \( \dot{m}_{\text{Tot}} \) is the total mass flow to the engine.

In the experiments and simulations, pure nitrogen is used as EGR. Both in the experiments and simulations, 20% EGR has been used. This means that the oxygen content in the oxidizer stream is about 18.6% on mass bases. If the exhaust gases from the research engine would be used instead of synthetic EGR, the EGR rate would be close to 40% in order to keep the oxygen level the same.

Figure 3 - Measured smoke number (left) and measured \( NO_x \) emissions in the diesel experiments with 50% engine load (right). In the EGR case, 20% EGR (pure \( N_2 \)) has been used.

5.2 Pressure and temperature fields

Measured and computed pressure curves are shown in the Figure 4. In the same figure also heat release rates are shown. It is seen that the measured and computed pressures are in good agreement. The 20% EGR case has lower heat release rate and hence lower pressure. The measured pressure curve is obtained with 0% EGR. The Miller cycle pressure curve is very close to the measured pressure curve. Computed mean and maximum gas temperatures are shown in the Figure 5. It is seen that 20% EGR lowers the maximum temperature by about 200K. The mean temperature is lowered also, at maximum about 80K. Miller cycle is seen to lower the average temperature throughout the combustion and expansion stroke whereas EGR lowered the mean temperature mainly during the most intense phase of combustion. On the other hand, Miller cycle does not affect the maximum temperature significantly.

Figure 6 shows the combustion regimes using simplified Phi-T map at the crank angle 24 after top dead centre. Also shown in the figure are the local temperatures and equivalence ratios. The sooting area (red area) is seen to be much larger in the 0% EGR case than in the 20 EGR case. It is also seen that the local equivalence ratios are very close to each other between 0% and 20% EGR cases. Hence, the reason for the different sooting tendencies is in the different local temperatures. The 20% EGR case has lower temperatures, so the soot peninsula in the Phi-T map is avoided. The 0% EGR case, on the other hand, has more combustion areas in the sooting peninsula. However, this computational result is contradictory to the experimental result seen in
the Figure 3 where much more soot is produced when EGR is used. In the Miller cycle plot the ambient gas temperature that has not been heated up by combustion is seen to be lower than in the other cases.

Figure 4 – Measured and computed pressure curves and heat release rates. The measured pressure is with 0% EGR.

Figure 5 – Computed mean and maximum temperatures.
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Figure 6 – Temperature (top), equivalence ratio (middle), and combustion regimes (bottom) without EGR (left), with 20% EGR (middle) or with Miller cycle (right) at the crank angle 24 after top dead center. The combustion regimes are plotted roughly according to the Phi-T maps. Red color indicates soot production area, light green corresponds to Low temperature combustion area and light blue means no combustion.

5.3 Phi-T maps of PAH and NOx

The Phi-T maps, or better T-Phi maps, were constructed using the chemical mechanism described earlier. Based on experimentally obtained pressure curves and temperature obtained from CFD simulations, the maps were constructed using a pressure of 80 bars and a residence time of 2 ms. The calculations were done using the closed reactor model in CHEMKIN 4. The reaction mechanism does not include heterogeneous reactions. Hence, the sum of PAH from pyrene to coronene was used to indicate the soot formation areas. In this case, when the experimental soot measurements are based on the smoke number, quantitative comparisons would not be possible even if a comprehensive soot mechanism was utilized.

In the calculations, the paraffinic HVO was modeled as n-heptane. The EN590 was modeled using a mixture of n-heptane, benzene and naphthalene. The molar composition of the EN590 model mixture was 65% n-heptane, 27% benzene and 8% naphthalene. On mass bases this corresponds to a fuel with 70 mass-% aliphatic hydrocarbons, 20 mass-% aromatics and 10 mass-% polyaromatics.

Figure 7 a-d shows Phi-T maps calculated for the two fuels with air as oxidizer. Superimposed on the maps are the Phi-T values in the CFD simulations of the engine. In the CFD simulations, the same overall hydrocarbon was used to describe the paraffinic hydrocarbon based fuel and the EN590. The figures show that at a crank angle of 20°, many of the computational cells are in the region where high concentrations of PAH are predicted. At this instance, there is not a big
difference between the fuels. At 60 ° the difference between the two fuels is clearer. For the n-heptane case, the branch of computational cells being fuel rich extends into the PAH formation area in such a way that the computed PAH mole fraction is approximately 10 times lower compared to the case where a mixture of n-heptane, benzene and naphthalene was used. However, it should be noted that the temperature in the most fuel rich cells are around 1800 K. Although an influence of the fuel mixture composition on the NO\textsubscript{x} formation is possible, the Phi-T maps do not reveal such a difference. Both in the n-heptane and in the n-heptane, benzene and naphthalene mixture case several of the cells in the CFD calculation is in the NO\textsubscript{x} formation zone at 60°.

Figures 8a-d shows corresponding Phi-T maps for the case when the diesel engine was run in EGR mode. In these runs the O\textsubscript{2} content of the oxidizer stream was 18.6 mass-%. The figures show that the in this case the peak temperature is lowered approximately 200 K. In this case too, the difference between the PAH levels in the Phi-T locations obtained in the CFD simulations is approximately a factor 10, being lower in the n-heptane case.

Figure 9a-d shows Phi-T maps for the case when the Miller cycle has been applied. The figure shows that compared to the standard case, the NO\textsubscript{x} producing region is slightly less entered. However, compared to the EGR case, a large fraction of the fluid inside the cylinder is entering the NO\textsubscript{x} producing region.

Based on Figure 7 and 9 a likely sooting tendency ranking is EN590/air & EN590/air+Miller > HVO/air & HVO/air+Miller > EN590/EGR > HVO/EGR. Based on the figure, there is no influence of the fuel quality on the NO\textsubscript{x} formation tendency. However, significantly lower NO\textsubscript{x} emissions can be expected using EGR. For the Miller case, no experimental data is available. Comparing with the results in Figure 3, one can conclude that for the NO\textsubscript{x} formation tendency the interpretation of the Phi-T maps agrees well with the measurements. For the sooting tendency, on the other hand, the results are contradicting. According to Figure 3, less smoke is formed in the air case compared to the EGR case. Based on this, the Phi-T maps are not very useful for predicting the sooting tendencies. However, these results should be reviewed critically, since the relation between the smoke number and the sum of PAH consisting of pyrene to corone may be debatable.
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Figure 7 - Phi-T maps of PAH and NO\textsubscript{x}. a) CA = 20º, n-heptane/air. b) CA = 60º, n-heptane/air.
c) CA = 20º, n-heptane, benzene, naphthalene/air, d) CA = 60º, n-heptane, benzene, naphthalene/air.
Superimposed a cell values from the CFD calculation with air.
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Figure 8 - Phi-T maps of PAH and NO. a) CA = 20º, n-heptane/EGR. b) CA = 60º, n-heptane/EGR. c) CA = 20º, n-heptane, benzene, naphthalene/EGR, d) CA = 60º, n-heptane, benzene, naphthalene/EGR. Superimposed a cell values from the CFD calculation with 20% EGR (pure N₂).
6. Conclusions

New measured engine data has been obtained from a heavy-duty diesel engine for off-road applications. The Miller cycle test showed that it lowers the mean temperature very effectively throughout the expansion stroke whereas EGR lowered the mean temperature only during the most intense phase of combustion. Maximum gas temperature was lowered more effectively by using EGR. The fuels used were the standard EN590 diesel fuel and a paraffinic hydrotreated vegetable oil (HVO) which has no aromatics in it. Different EGR rates were also used in the experiments. The effects of EGR and those from the paraffinic diesel fuel have also been used in the creation of Phi-T maps by detailed chemistry calculations. CFD was used to analyze the local combustion conditions in the combustion chamber by utilizing the created Phi-T maps. This combination of detailed kinetic calculations, the new measured data, and the CFD analysis was found valuable in analyzing the Phi-T maps together with the measured engine emissions.

Combining Phi-T maps, superimposed with Phi-T values of computational cells in CFD calculations, with the information about the critical mixing time obtained from the kinetic mixing
calculations, is likely a good way to qualitatively predict sooting tendencies. If the sooting peninsula is completely avoided, sooting is unlikely. If the sooting peninsula is entered during the combustion cycle, complete mixing should be obtained before entering temperatures too low for PAH (and soot) oxidation. Tracking the fraction of cells that have been in the sooting area, and that still are fuel rich when the local temperature drops below 1300K is probably a useful approach.

7. References

[1] Kamimoto, T., and Bae, M., High combustion temperature for the reduction of particulate in diesel engines, SAE paper 880423, 1988