INTERNAL COMBUSTION ENGINE SOOT AND NOx FORMATION SIMULATION

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Abstract

The reduction of NOx and soot emissions are, beside the improvement of fuel efficiency, the main goals of modern diesel engines development. Advanced experimental and simulation techniques are used in order to clarify the spray break-up and pollutant formation mechanisms. To simulate the details of the physical and chemical phenomena that define the combustion process, Computational Fluid Dynamics (CFD) is the most appropriate simulation technique. In the present work, a CFD simulation of a diesel engine fuel injection process is performed. It includes the piston motion, the air-fuel mixing and the combustion simulation. The focus was on the NOx and soot formation processes. The OpenFOAM software toolbox was used for the purpose. The Huh model was used to simulate the fuel injection. The chemical reactions were tracked with a 15 specie Chemkin type reaction model. A modified Fusco model was used for soot formation and oxidation. After the development of the cylinder calculation mesh, the models were tuned. The simulation results were compared with experimental data. Finally, several split injection patterns were tested in order to evaluate its influence on pollutants formation.

1 Introduction

The transport sector has a very important role in the modern society and it is mostly based on the power provided by internal combustion engines. However, the burning of fossil fuels contributes to the fuel and pollution crisis. Some authors suspect the connection of the global warming and the CO_2 emissions. The diesel engine is one of the most effective devices for conversion of the fuel chemical energy to mechanical energy. It is often used as a propulsion systems in transport means. Modern systems like variable injection timing, variable exhaust valve operation and exhaust gas recirculation allow to the engine operation flexibility and further emission and fuel consumption reduction. To develop, tune and test the various combinations of the operation parameters allowed by this new systems, mathematical modeling and computer simulation are very useful because they allow to check many different parameters. However, computer simulations are always used in combination with experimental research in order to validate the calculation results.

CFD (Computational Fluid Dynamics) simulations are the most complex level of mathematical models for engine simulation. However, they are necessary in some cases when a high level of detail is needed. In particular it is necessary if the geometry influence on the performances has to be evaluated. CFD simulations are necessary also for pollutant formation calculation since the chemical rates are highly influenced by the local temperature variations[1]. There are different projects and software that allow CFD analysis of engine processes. OpenFOAM [2] is an open source, free CFD collection of solvers and libraries written in C++. For its availability, flexibility and the collaboration between users it is a good platform to use to approach uncommon CFD problems.

The main pollutants from diesel engines are NOx (nitrogen oxides) and soot. NOx is the denomination for several combinations of nitrogen and oxygen atoms including NO, NO_2, N_2O, N_2O_3 and N_2O_5. Most of them are toxic. NO represents more then 90% of all the nitrogen oxides in diesel combustion products. For that reason only the production of this specie is analyzed. NO is usually calculated with the Zeldovich set of kinetic equations [3], [4], [5]. Soot is a more complex problem. Soot formation is a chemical process at the very beginning, when fuel molecules are recombined in molecules that represent soot precursors. In the later phase soot particles grow by physical agglomeration. The total amount of soot is given by the difference of the processes of soot formation and soot oxidation [3], [4], [5], [6], [7]. Beside the unpleasant smell of the hydrocarbons absorbed by the soot, and the fact that it is visible in higher concentrations, the main problem of soot is the fact that it can cause cancer. To limit these negative influences, legislation dictates the emission standards that limit the highest emission levels.

The reduction of NOx and soot emissions are, beside the improvement of fuel efficiency, the main development goals of modern diesel engines.

In the present paper a CFD simulation of a direct injection diesel engine was performed. Different split injection patterns, including pilot injection and post injection were analyzed in particular and their influence on the soot and nitrogen oxides emissions.

2 Mathematical model

The 3D numerical simulations are based on the laws of conservation. The conservation of mass is described by equation (1):

$$\frac{\partial \rho}{\partial t} + \mathrm{div}(\rho \mathbf{V}) = \rho_{evap} \tag{1}$$

where ρ is the density, t is the time, $\mathbf{V}$ is the velocity vector and $_{evap}$ stands for evaporation.

Similar equations are used to describe the momentum conservation in the 3 Cartesian coordinates and the conservation of energy. Since chemical reactions are analyzed, a similar equation is used to track the transportation of each chemical species. In the simulations the RNG k-ε turbulence model is used, which uses similar equations too. All these equations have the same structure which can be described by equation (2):

$$\frac{\partial(\rho \Phi)}{\partial t} + \mathrm{div}(\rho \Phi \mathbf{V}) = \mathrm{div}(\Gamma \mathrm{grad}\Phi) + S \tag{2}$$

where ρ is the density, Φ is a generic property of the fluid, t is time, $\mathbf{V}$ is the velocity vector and S is the source or sink of the property.

The first term describes the change of the property in time, the second term describes the property transport with the mechanism of convection. The first right hand side term describes the diffusion transport of the property and the last term stands for the source or the sink of the property. Since the equations describe the transport of a property in the domain they are sometimes called transport equations [8].

For fuel jet atomisation the Huh model was used. This model couples the effects of two phenomena relevant in spray atomisation, namely, the turbulent fluctuations in the liquid jet, and the unstable wave growth at the jet surface by aerodynamic effects between the jet and surrounding gas at their interface. The conceptual picture of the atomisation process takes it to proceed in two stages:

1. Turbulence developed in the nozzle hole induces initial perturbations on the jet surface when it leaves the hole,
2. Once the perturbations have reached a certain level, they grow by the action of aerodynamic forces until they become detached from the jet surface as droplets;

In the model, firstly the length and time scales of atomization are identified, and then they are used to determine the breakup rate, droplet size distribution and spray cone angle. Further spray model details are given in [9].

In order to simulate the chemical reactions, a chemical scheme with 15 species and 39 reactions was used. It includes the Zeldovich mechanism for the calculation of NO:

$$N_2 + O \longleftrightarrow NO + N \tag{3}$$

$$N + O_2 \longleftrightarrow NO + O \tag{4}$$

$$N + OH \longleftrightarrow NO + H \tag{5}$$

The base for soot calculation is a model proposed by Fusco et al. [7]. It is a phenomenological soot creation model that incorporates, via global rate expressions, the physical processes of pyrolysis, particle inception, surface growth, particle coagulation and oxidation, as well as global reaction steps for intermediate species formation and oxidation. A schematic diagram of this soot model processes is shown in Figure 1. The intermediate reactions are reported in [5], [6] and [7]. Finally, the soot number density [N_p], the precursor radical density [VR], the growth specie density [C_2H_2] and the soot volume fraction [υ_{fR}] are calculated as in equations (6)-(9):

$$\frac{d\lfloor N_p \rfloor}{dt} + \mathit{\Delta}\left(\Phi \cdot N_p\right) = N_a \cdot r_5 - r_8 \tag{6}$$

$$\frac{d[VR]}{dt} + \mathit{\Delta}\left(\Phi \cdot VR\right) = r_1 - r_3 - r_5 \tag{7}$$

$$\frac{d[C_2H_2]}{dt} + \Delta\left(\Phi \cdot C_2H_2\right) = +r_2 - r_4 - r_6 \tag{8}$$

$$\frac{d\lfloor \upsilon_{fR} \rfloor}{dt} + \Delta\left(\Phi \cdot \upsilon_{fR}\right) = \frac{1}{\rho}\left(r_5 MW_{VR} + r_6 MW_C - r_7 MW_C\right) \tag{9}$$

where t is the time, Φ is the surface flux, ρ is the density, N_a is the Avogadro's constant, r_1 to r_8 are the reaction rates.

3 Numerical simulation

The simulated engine was the MAN D 0826 LOH15 mounted on the test bed in the internal combustion engine laboratory of the Faculty of engineering of the University of Ljubljana. It is a classic direct injection engine used for truck or bus propulsion. It features a camshaft driven fuel injection pump. This engine was chosen because there were many data available about it and there were detailed experimental measurements performed on it. The engine basic characteristics are presented in table 1. The engine mounted on the test bed in the laboratory is shown on figure 2.

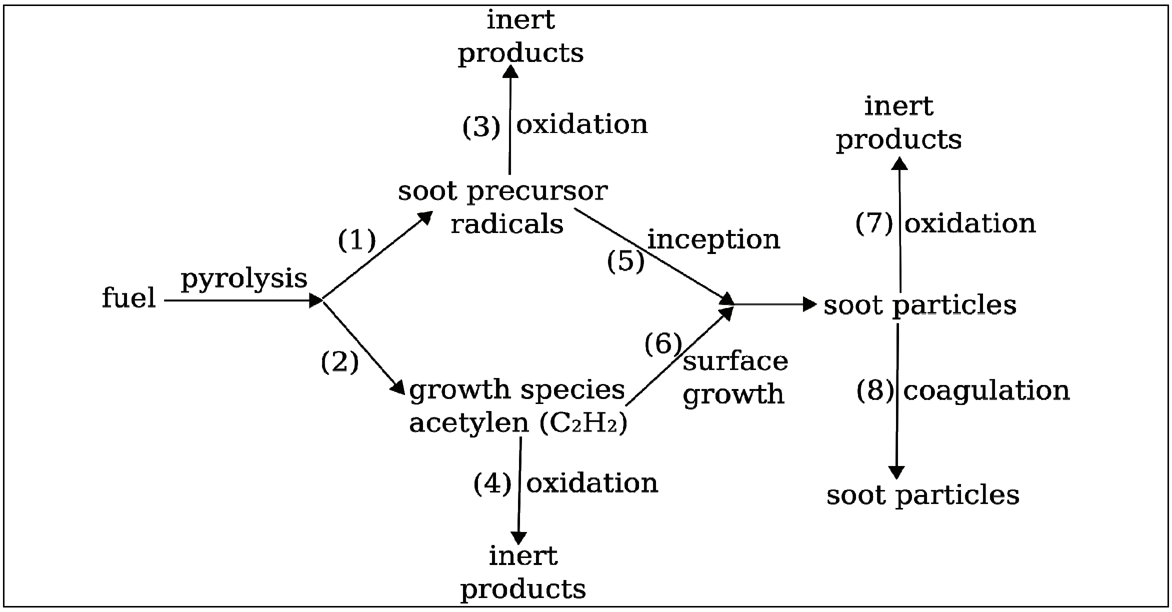

Figure 1: The Fusco soot model reaction scheme [2]

Table 1: Basic MAN D 0826 LOH15 engine characteristics

Swept Volume	6,87 l dm^3
Number of Cylinders	6
Power	160 kW
Bore	0.108 m
Stroke	0.125 m
Capacity (1 cylinder)	0.00114511 m^3
Compression ratio	18
Connecting rod length	0.1872 m

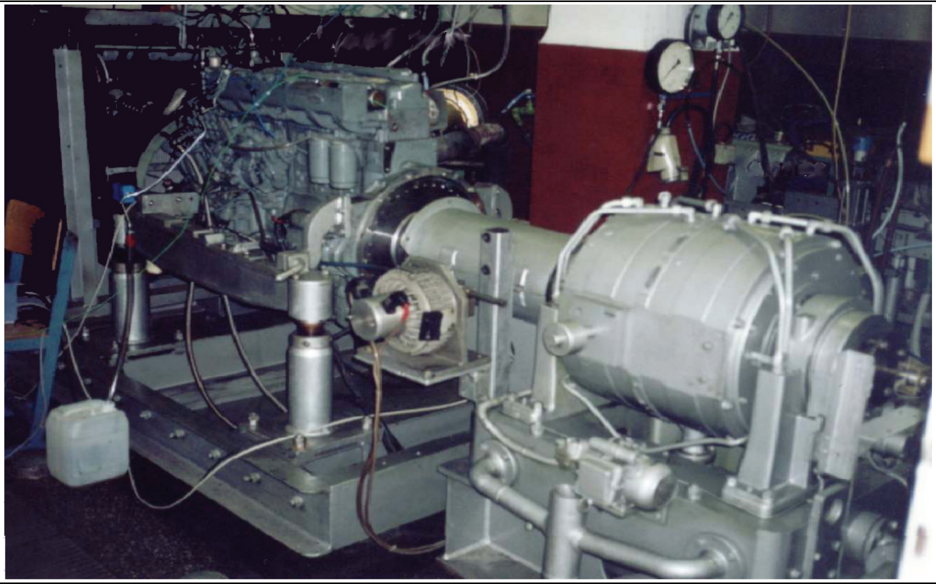

Figure 2: The engine mounted on the test bed

A calculation mesh of the cylinder volume was built. A special feature of the engine cylinder CFD simulation is the variation of the domain volume. In order to keep the aspect ratio of the calculation cells constant the layer addition/removal strategy was used. The calculation mesh of the cylinder is shown in figure 3. The OpenFOAM model was set for the simulation of the injection, combustion and pollutant formation. The initial data consist, besides of the calculation mesh, of calculation details, engine geometry data, injection details, boundary conditions, turbulence model details, spray model details, fuel properties and chemistry scheme data.

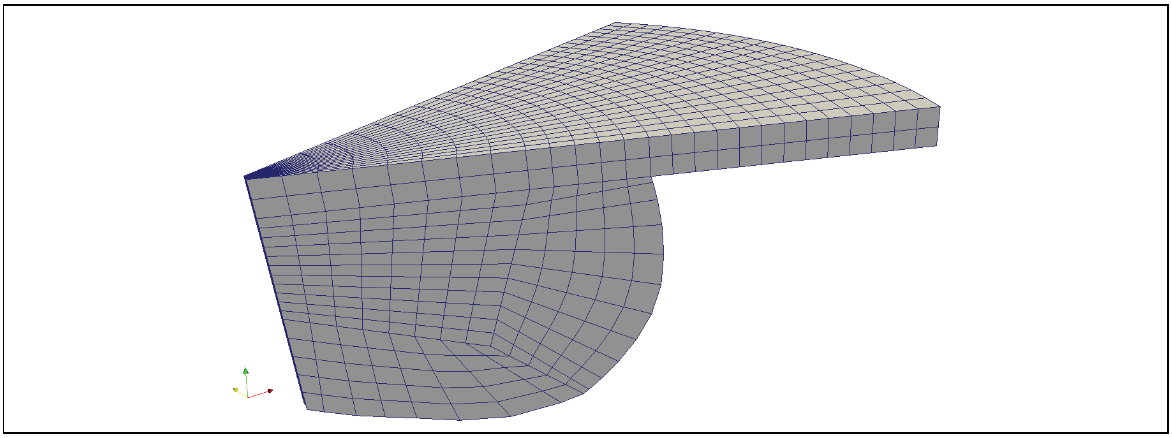

Figure 3: The calculation mesh of the cylinder

Different regimes were simulated, and the the results of the simulations were in good agreement with the experimentally obtained results. In particular the cylinder pressure history obtained was very similar as far as the maximum level and shape to that obtained by experimental measurement. The nitrogen oxides emission simulation results are somewhat less in agreement with experimental engine out NOx emissions. The differences between the simulations and the measurements are from 10% to 50 % depending of the regime simulated. The soot simulation results are less accurate, since they differ from the experimentally measured results by several orders of magnitude. However, the trends of the pollutant formation simulations reflect those of the experimental measurements. This means that a measured increase of NO or soot emission for some engine parameter change is well reflected by the increase of the simulated pollutant production. Hence the simulation is considered to be sufficiently accurate for further qualitative engine analysis, keeping in mind that the absolute emission values can not be trusted.

An upgrade of such an engine would be the installation of a common rail injection system which would allow higher flexibility and different injection patterns. Such injection strategies are used in first order to allow a more fluid engine run with less vibration. Beside it, some investigations show that such strategies are useful for emissions reductions, especially for soot emission reduction [10], [11].

In the current paper 6 injection patterns are tested. The used patterns are the same as in [11], figure 4.

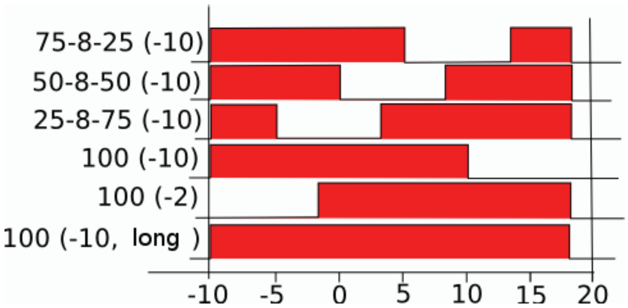

Figure 4: The injection patterns

The injection is performed in 1 or 2 phases of different duration. The injected fuel mass is the same for all the cases. The first strategy consists of two phases, the first starts 10º before the top dead course (TDC). It lasts until 5º after top dead course. Then there are 8º without injection (pause, break), after which the second injection phase starts at 13º and lasts until 18º after TDC. In the first phase, 75% of the fuel amount is injected and in the second the remaining 25%. The second and the third strategy are defined in similar manner. The remaining three strategies consist of one injection phase, without breaks, with different starting points and durations as shown in figure 4. The denomination of the strategies consists of the percent of fuel injected in the first phase, the duration of the pause between the phases and the percent of fuel injected in the second phase if it exists. In brackets, there is the crank shaft angle of the start of injection respect to the TDC.

4 Results

A characteristic result of a CFD numerical simulation allows the insight into the spatial distribution of some phenomena. An example of such a result is presented in figure 5. The distribution of the isosurface of 2000 ppm of NO and the soot cloud are presented for the moment of 12º after TDC. However, such results do not allow to easy compare some parameters such as pollutant quantities for all the cases simulated. Hence, the domain integrated quantities for rate of heat release (RoHR), cylinder pressure, cylinder temperature, fuel vapour concentration, NO concentration and soot concentration are calculated and presented in figures 5 - 10.

In figure 6 it can be seen how different injection strategies influence the heat release rate. The initial hump on the curves indicates how the model reproduces the fast combustion of the fuel that arrived to be mixed with air before ignition. The hump position is the consequence of the start of injection. A later start of injection for the case 100(-2) results in a slightly lower heat release rate. The cases 75-8-25(-10), 50-8-50(-10), 25-8-75(-10) and 100(-10) have in common a large amount of fuel injected in an early stage and it results in an intensive heat release in the early phase. The last case, 100(-10, long), is characterized by the long injection and hence a lower heat release rate.

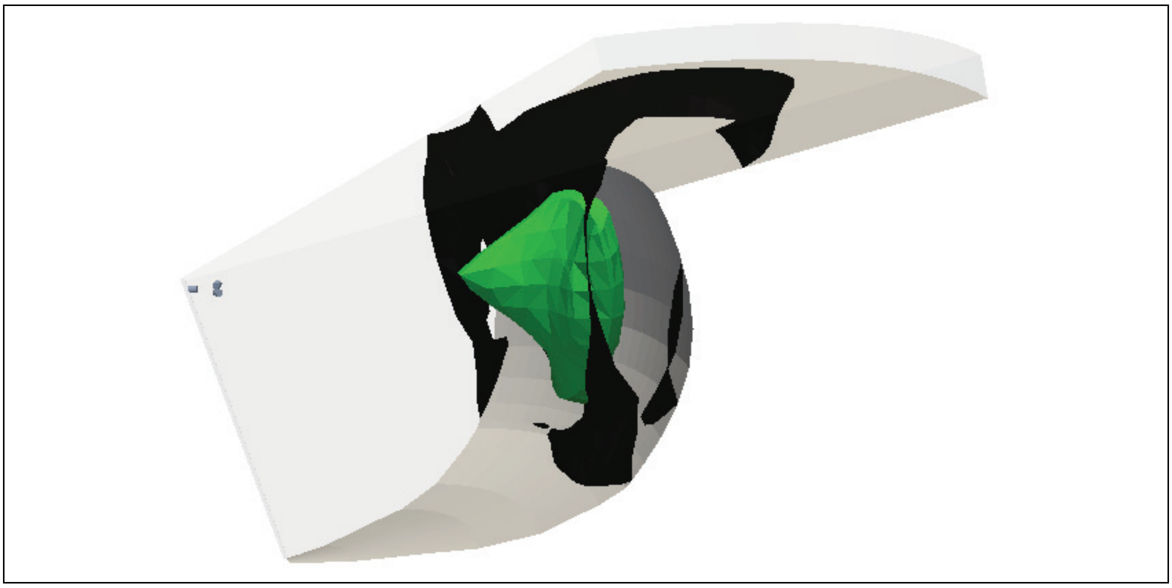

Figure 5: The distribution of the isosurface of 2000 ppm of NO and the soot cloud are presented for the moment of 12º after TDC

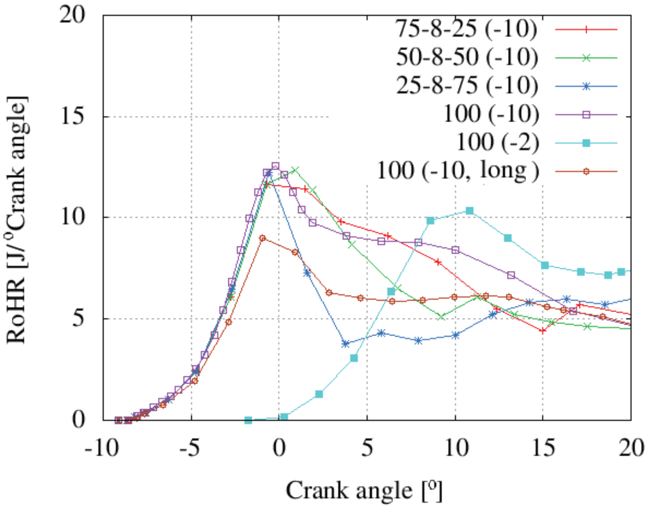

Figure 6: Rate of heat release

In figure 7 it can be seen how the heat release is reflected by the pressure rise in the cylinder in dependence of the injection strategy. The strategy 50-8-50(-10) results with the highest maximal pressure and the 100(-2) with the lowest. The surface under the curves is a measure of the indicated work. It is clear that to achieve the same engine power it would be necessary for the surfaces to be same. If we want to achieve a bigger surface we should inject more fuel for some injection strategies. For these strategies hence the fuel efficiency would be lower. The surface is biggest for the case 100(-10), which means that the fuel efficiency is best for this case. Usually an early injection is related to the improvement of the fuel efficiency, which is confirmed by this analysis. However, it is related to the increase of maximal temperatures and NO emissions too.

In figure 8 it is presented how the different injection strategies influence the average cylinder temperature. Temperature is an important parameter since it has a strong influence on the nitrogen oxides formation and on the formation and oxidation of soot. The local temperature is the one that influences the rates of the mentioned reactions. It can be much higher than the average temperature. However the average temperature is also useful as a measure of pollutant formation tendency. The highest temperature is achieved for the cases with the early injection such as 100(-10) and 75-8-25(-10) and the lowest for the case with late injection 100(-2), but also for the multiphase injection case 25-8-75(-10).

In figure 9, the average fuel mass fraction is presented for the different injection patterns. The local fuel concentration has a great influence on soot formation since soot is created in the fuel rich regions as a reaction between certain hydrocarbon molecules. The average value can also be useful as a measure of tendency to soot formation. In the figure it can be seen that the mass fraction increases due to fuel injection and evaporation. In one point the fuel fraction begins to decrease. It is the moment when the chemical reactions that consume the fuel become faster then fuel evaporation. It can be noticed the double maximum for the cases with injection in two phases. It can also be concluded that injection in more phases results with a lower maximal levels of fuel concentration in the cylinder which could lead to a lower soot formation tendency.

In figure 10 it is shown the influence of the injection patterns on nitrogen oxide formation. For all the cases it can be seen a characteristic sharp increase during the combustion process. The NO is created in the regions of the flame with the local temperature of more then 2000 K. After this phase the quantity of NO remains constant because the temperature drops below 2000 K as a consequence of expansion and heat transfer. The highest mass fraction of 0.0006 kg/kg of NO is reached for the cases 75-8-25(-10), 50-8-50(-10) and 100(-10). The lowest mass fraction is found for the late injection case 100(-2). From the analysis it can be confirmed the correlation between NO formation and cylinder temperature. The fastest NO concentration growth is achieved for the strategy and period with the highest temperatures in the cylinder, between 0 and 20º after TDC.

In figure 11 it is presented the injection strategy influence on soot concentration. For all the cases it can be seen a characteristic trend of soot concentration. The initial phase of intensive soot formation is a consequence of the combustion in a region of high fuel concentration. After it follows the oxidation phase that lasts until the temperature drops under a certain temperature. From the analysis it follows that the maximal soot concentrations are obtained for the cases with early fuel injection.

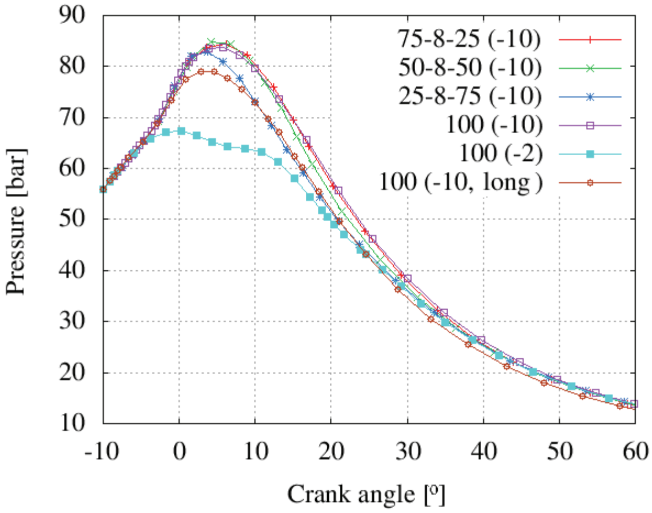

Figure 7: Cylinder pressure

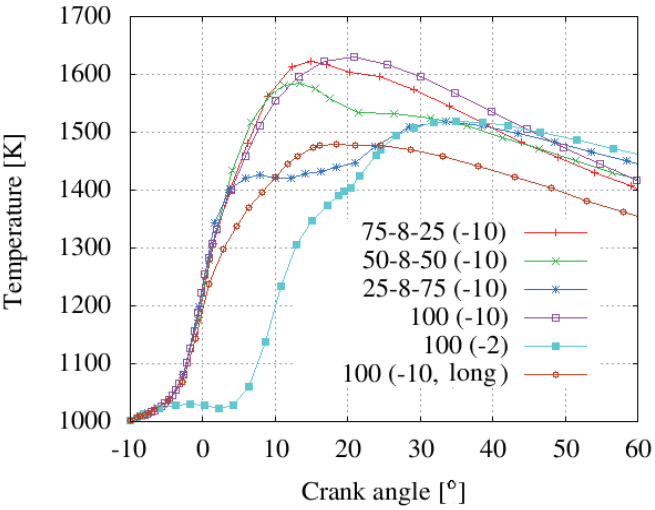

Figure 8: Cylinder temperature

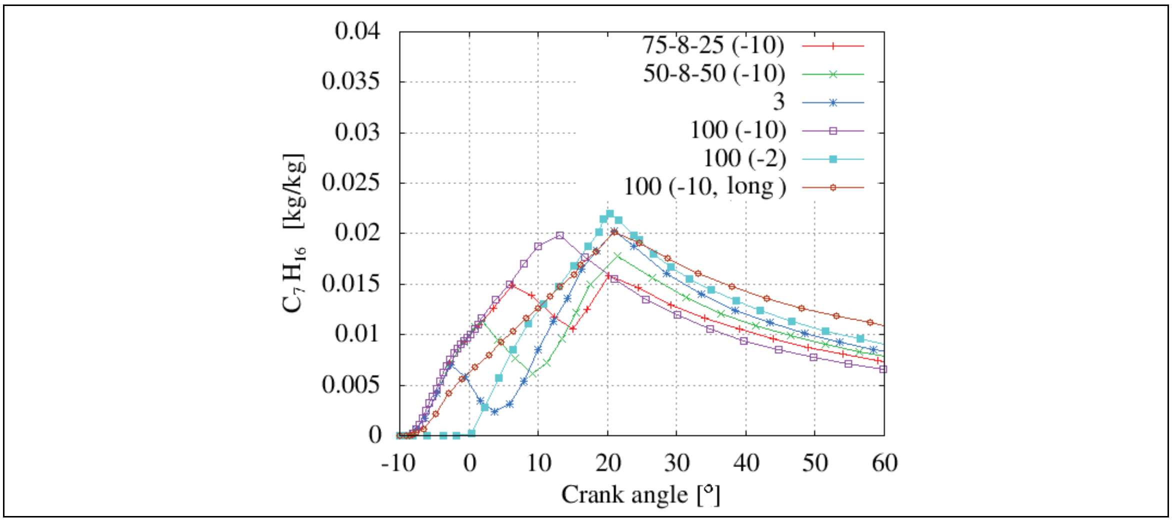

Figure 9: Fuel vapour mass fraction

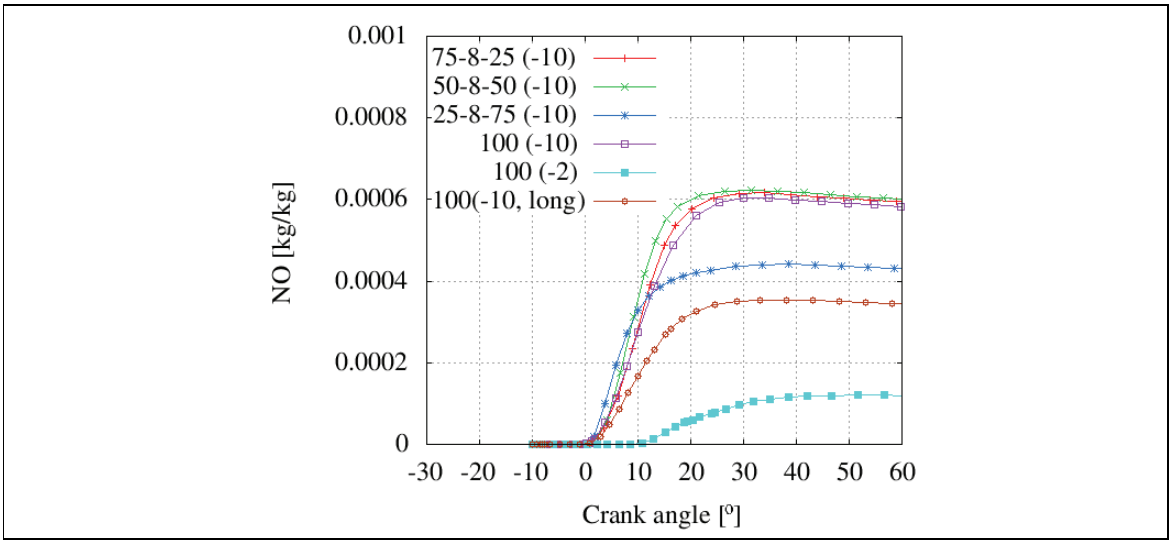

Figure 10: NO mass fraction

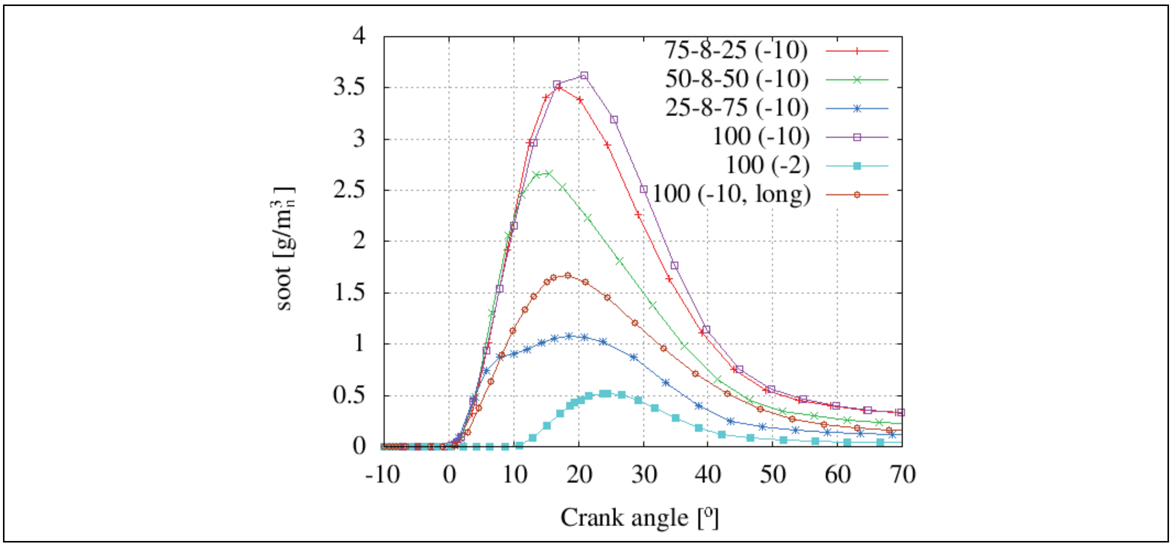

Figure 11: Soot concentration

5 Conclusion

In the present paper, a CFD analysis of the injection, combustion and pollutant formation in a diesel engine has been performed. The OpenFOAM software is well suited for such analysis and it is relatively simple to implement new models. The Huh spray model showed good results in earlier works [9]. In the present work there were no experimental measurements of the spray parameters, but the pressure history of the simulated engine is very similar to the experimental one, and hence it can be concluded that the spray model is good enough for the purpose.

The chemistry model with 15 species was chosen as a compromise between simpler models that have less detail and do not have the NO formation models and of more complex models that slow down the calculation considerably and make it less stable. The included Zeldovich's NO formation model is very common, and the results for NO mass fraction conform very well with the experimental measurements. However, it was noticed that the chemistry model has a great influence on the results and hence it is considered as one of the main fields for further investigations.

Another problem with the simulation was the uncertainty of some experimental details necessary for setting the initial conditions (injection pressure history, nozzle geometry, injection flow, needle lift timing..). These data do influence the final results somewhat. To overcome this problem, the same data were used for all the injection cases and the injection flow pattern was the only variated parameter and only trends have been observed.

The soot modeling is still in the phase of development. The simulated soot quantities differ from the experimental quantities by several orders of magnitude. However, the trends showed to be in agreement with the measurements in earlier works ([5], [7]) and this is good enough to analyze the influence of different injection patterns.

The insight offered by CFD is very detailed. All the intermediate parameters can be simulated. Here the rate of heat release, the pressure, temperature, and fuel vapour concentration were selected as most influential for pollutant simulation. Late injection is characterized by lower maximal temperatures and hence by lowest emission levels. However, also the resulting cylinder pressure is considerably lower which would result with lower power output or higher specific consumption. The cases with injection that starts at the moment of -10 degree TDC show that earlier fuel injections offer higher pressure levels, but at the expense of higher temperatures and higher pollutants production. The cases with multiple injection result with lower maximal fuel vapour concentrations, and hence lower soot levels compared to the continuos injection cases. The case 25-8-75 (-10) appears to be the best compromise between maximum cylinder pressure (power), NO and soot levels.

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