3D-CFD SIMULATION OF DI-DIESEL ENGINE COMBUSTION AND POLLUTANT FORMATION

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Abstract: *Three-dimensional Computational Fluid Dynamics (3D-CFD) is applied to study combustion and pollutant formation in a high-speed DI-diesel engine. Auto-ignition is modeled on the basis of tabulated detailed chemical kinetic calculation results. Premixed flame and diffusion combustion are simulated by adopting a coherent flame modeling approach. High temperature oxidation is approximated by a three-step mechanism combined with an equilibrium chemistry approach. The simulation of thermal NO formation is based on the well-known Zeldovich mechanism, soot formation and oxidation processes are modeled on the basis of a reduced chemical kinetics soot model. The set of models is implemented in the CFD code AVL FIRE and is used to study the impact of variations of in-cylinder swirl, start-of-injection, injection pressure and residual gas content on the engine combustion and emission characteristics. The focus of the study is on the analysis and assessment of the sensitivity of the adopted combustion and emission modeling approach on the investigated combustion system parameter variations. Quantitative assessment of the model performance is made via comparison of the calculation results with data from cylinder pressure indication and tail-pipe emission measurements. The comparison between calculated and measured results shows good agreement for both the in-cylinder pressure traces and the pollutant emission trends for the investigated combustion system parameter variations.*

Keywords: CFD, diesel engine, combustion, pollutants

INTRODUCTION

DI-diesel engine performance and emission characteristics are mainly governed by in-cylinder flow, fuel spray injection and combustion. A better understanding of the interaction of turbulent in-cylinder flow, liquid fuel spray propagation as well as auto-ignition and combustion is hence a major prerequisite to optimize DI-diesel engine combustion systems to meet the increasing legislative and environmental demands regarding fuel efficiency and pollutant emissions. Due to the strong spatial and temporal inhomogeneities of the in-cylinder temperature and mixture composition fields, however, conventional cylinder-pressure indication and tail-pipe emission measurements only provide limited insight into the relation of the injection/combustion system parameters and the overall engine performance and emission characteristics. Hence, CFD simulation of in-cylinder spray propagation, combustion and pollutant formation processes is becoming an increasingly indispensable tool in DI-diesel engine combustion system development.

The accuracy of the CFD calculation results of DI-diesel engine combustion and pollutant formation largely depends on the predictive accuracy of the mathematical models adopted for liquid fuel spray injection, auto-ignition and combustion, as well as on the models used for calculation of NO and soot formation/oxidation. In the last two decades a variety of combustion models has been proposed and applied to different DI-diesel engine analysis and optimization studies. Models of different levels of complexity, such as eddy-break-up type models [1], [2], approaches based upon adoption of laminar/turbulent characteristic time-scales [3], or models following the concept of representative interactive flamelets [4] have been used to study combustion and pollutant formation in DI-diesel

engines. Due to its universality to capture both conventional and alternative HCCI-type combustion regimes, the ECFM-3Z combustion model [5] is adopted in the present study, suitably coupled with a model for the formation of thermal/prompt NO [6] and linked to a novel chemical kinetics based advanced soot formation/oxidation approach.

The above set of combustion and pollutant formation models forms an integral part of the CFD code FIRE [7]. In the present work the combustion/emission model suite is used in combination with the well-established spray formation/propagation models available in FIRE for the analysis of the impact of combustion system parameter variations on the performance and pollutant formation characteristics in a DI-diesel research engine. The study is conducted for a number of variations of in-cylinder swirl intensity, start of injection, injection pressure and residual gas content for a selected part load operating point. The major focus of the work is on the analysis of the adopted CFD modeling approach with respect to its predictive accuracy and reliability to reflect the impact of combustion system parameter variations on the engine combustion and emission characteristics. Validation of the sensitivity of the combustion and pollutant formation models on the investigated combustion system parameter variations is achieved via comparison of the predicted in-cylinder pressure traces and pollutant emissions with engine measurement data.

MODELING

The commercial CFD code FIRE is used throughout the present study. In the following, the basics of the FIRE solver and the related solution algorithms as well as information on the spray, combustion and pollutant formation models adopted in the present work are briefly presented.

Flow Solver and Solution Algorithm

The CFD code FIRE solves the general conservation equations of mass, momentum and enthalpy plus transport equations for turbulence, conservation of chemical species and additional scalar quantities, such as e.g. mixture fraction, reaction progress variable, flame surface density, etc. The solution method is based on a fully conservative finite-volume approach. All dependent variables for momentum, pressure, density, turbulent kinetic energy, dissipation rate, and scalar quantities, such as e.g. chemical species, are evaluated at the centers of the computational cells [8]. Cell-face based connectivity and interpolation practices for gradients and cell-face values are used to accommodate unstructured moving grids with general polyhedral cells. A second-order midpoint rule is used for integral approximation and a second order linear approximation for any value at the cell-face. A diffusion term is incorporated into the surface integral source after employment of the special interpolation practice. For discretization of the convection term a second order accurate scheme is adopted. The rate of change is discretized by using an Euler implicit scheme. The overall solution procedure is iterative and is based on the Semi-Implicit Method for Pressure-Linked Equations algorithm (SIMPLE) applicable to turbulent flows at all speeds even including super-sonic flows. For solving the large sets of linear equation systems evolving from the discretization of the governing equations, an efficient preconditioned conjugate gradient method is adopted. For execution on multi-processor hardware, a domain decomposition parallelization approach is employed, enabling efficient solution of flow problems comprising of a large number of computational cells.

Fuel Spray Propagation

Propagation of liquid fuel sprays is modeled according to the Lagrangian discrete droplet method [9]. The continuous gas-phase is described by the standard Eulerian conservation equations, the transport of the dispersed fuel phase is calculated by tracking the trajectories of a large number of representative parcels. A parcel consists of a number of droplets with all the droplets within one parcel having the same physical properties and behaving equally when they move, break up, evaporate and interact with the combustion chamber walls. The coupling between the liquid and the gaseous phases is achieved by source term exchange for mass, momentum, energy and turbulence. Different sub-models account for

the effects of turbulent dispersion, coalescence, evaporation, wall interaction and droplet primary and secondary break up [10]. In the present study the blob-injection method in combination with the WAVE break-up model is used to model the primary atomization region and the secondary droplet break-up downstream of the injector. The value of the break-up model parameter is selected to fit the experimental spray propagation and combustion characteristics.

Ignition and Combustion

For modeling compression-ignition combustion the three-zone extended coherent flame model (ECFM-3Z) is used [5]. The ECFM-3Z distinguishes between the three major regimes relevant during diesel combustion, namely auto-ignition, premixed flame and non-premixed diffusion combustion. The auto-ignition pre-reactions are calculated within the premixed charge, with the ignition delay governed by the local temperature, pressure, fuel/air equivalence ratio and the amount of residual gas. Local auto-ignition is followed by premixed combustion in the fuel/air/residual gas charge formed during the time period between start-of-injection and auto-ignition onset. The third regime is the one of diffusion combustion where the reaction takes place in a thin zone which separates fuel and oxidizer. In the ECFM-3Z it is assumed that the chemical time in the reaction zone is much smaller than the time needed for the diffusion process. Therefore the rate of reaction during diffusion combustion is determined entirely by the intermixing of fuel and oxidizer. The amount of mixing is computed based upon a characteristic time-scale obtained from the solution of the k-ε turbulence model.

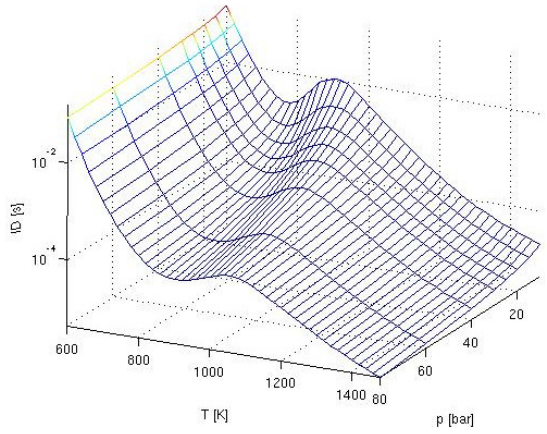

Fig. 1. Tabulated ignition delay time as a function of temperature and pressure

For the prediction of the auto-ignition process tabulated values of the ignition-delay time are used which are created based on a complex n-Heptane chemical reaction mechanism [11]. The auto-ignition data values are stored in a table as function of the parameters pressure, temperature, fuel/air equivalence ratio and residual gas content (Fig. 1.). The range of these parameters is chosen to cover the relevant conditions prior to combustion, i.e. pressure from 10 to 200 bar, temperature from 600 to 1500 K, equivalence ratio from 0.3 to 3.0 and residual gas mass fraction from 0 to 90%. During the CFD calculation the look-up table is accessed via a fast interpolation procedure ensuring minimized calculation time. For the actual determination of the auto-ignition delay time in the CFD simulation, a transport equation for an auto-ignition indicator species is solved with the formation rate derived from the tabulated values. Once the local value of the indicator species reaches a value of unity, the auto-ignition is initiated. Fuel consumption is then controlled by a small characteristic chemical time-scale which ensures rapid combustion after auto-ignition [12].

The hydrocarbon oxidation process during high temperature combustion is separated into three major reaction steps. First, the fuel is partly oxidized to CO and to CO_2, followed by CO oxidation and finally a post-flame equilibrium chemistry approach is applied which results in the final species concentrations. The adopted combustion reactions cover the relevant range of mixture composition from lean to rich and the different levels of residual gas content. In addition to the amount of heat that is released within the reaction zone the present reaction treatment provides the relevant information about all minor species which are important for the subsequent calculation of the NO formation process.

Pollutant Formation

NO Formation

The thermal NO formation is modeled by the widely accepted Zeldovich mechanism, adopting an overall NO formation rate for the three thermal reactions according to [13]. The concentration of O atoms and the free radicals OH appearing in the overall NO formation rate are based upon the radical concentrations provided by the high temperature oxidation process [6]. Under conventional diesel engine operating conditions thermal NO formation is considered to be the dominating source of NO emissions. Under high EGR conditions prompt NO might also contribute to the overall NO emission level. Hence, prompt NO formation is taken into account in the present work. The model used in the present study to predict prompt NO formation follows the approach proposed by De Soete [14].

Soot Formation

The soot model adopted in the present study is based upon a detailed chemical reaction scheme for the calculation of soot formation and oxidation [15], [16]. It combines the mechanisms of formation of polyaromatic hydrocarbons, polyynes, two mechanisms of soot precursor formation due to condensation of polyaromatic and polyyne molecules, soot particle growth by the reactions of the HACA mechanism and polyyne molecule addition, the mechanism of acetylene pyrolysis and pure carbon cluster formation, as well as the reactions of hydrocarbon oxidation. The complete detailed kinetic scheme of the soot formation process incorporates 1850 gas-phase reactions, 186 species and 100 heterogeneous reactions with participation of four ensembles of micro-heterogeneous particles of different types. The current model implemented in FIRE contains a reduced number of species and reactions and has been developed on the basis of the above described detailed kinetic mechanism in order to provide a computationally efficient kinetic overall soot model [7].

ENGINE ANALYSIS

The engine modeled in the present study is a single-cylinder research engine with electro-hydraulic valve actuation (EHVA) and intake ports with swirl flaps. The cylinder head is designed with an intake split port, comprising helical and neutral ports guided to the first intake valve and a tangential port at the second intake valve in order to control the charge motion in the combustion bowl via flaps. By continuously closing the flap in the neutral port the swirl is adjusted in a range between 1.7 up to 2.9, in case the flap in the tangential port is additionally closed the swirl can be continuously increased up to a level of 4.5. Control of the exhaust gas recirculation (EGR) is achieved by both an external EGR system and in a highly dynamic way by the EHVA system comprising different modes of internal EGR. Fuel injection into the combustion chamber is achieved via a Piezo Common Rail system with an injection pressure to be chosen between 250 bar and 1600 bar. The main engine and injection system data are summarized in Tab. 1.

Bore	85 mm
Stroke	94 mm
Displacement	533.4 cm^3
Compression ratio	16:1
Injection system	BOSCH Piezo CR
Number of injection holes	8

Tab. 1. Engine and injection system data

Following the general practice for 3D-CFD based analysis of DI-diesel combustion systems, only the high pressure cycle, i.e. the crank-angle position between intake valve closing and exhaust valve opening is modeled in the calculation. Due to the symmetric arrangement of the ω-shaped piston bowl,

the calculations are performed for an engine segment model, with the computational domain covering the cylinder/piston bowl configuration around one single fuel spray assuming cyclic symmetry.

The gas-side initial conditions at the time of inlet valve closure, i.e. in-cylinder pressure, temperature and residual gas mass fraction, as well as the wall temperature boundary conditions are obtained from a 1D cycle-simulation, in the present study adopting the 1D-CFD code BOOST [17]. A solid body rotation of the in-cylinder flow field at the time of inlet-valve closure is prescribed in the engine segment calculations, with the swirl levels and turbulence intensities extracted from preceding 3D-CFD calculations of the entire intake and compression strokes. The standard two-equation k-ε turbulence model together with the logarithmic law of the wall is used for both the full and sector model calculations. The resulting swirl level and turbulence intensities at injection timing hence obtained for the sector mesh closely resemble the corresponding flow characteristics in the full engine model for the operating conditions investigated in the present study.

The fuel side boundary conditions, i.e. hydraulic injection timing and injection rates for the different injection pressure levels are obtained on the basis of hydraulic simulation results adopting the 1D-tool HYDSIM. Parameterization of the hydraulic model is conducted on the basis of injector flow measurements and selected three-dimensional nozzle flow simulations [18].

For the purpose of the present study of analyzing and assessing the sensitivity of the adopted combustion and emission models to combustion system parameter variations, the 3D-CFD calculations are performed for a selected part load operating point. For the speed/load point under consideration a considerable number of combustion system parameter variations is performed, comprising variations of start of injection (SOI), residual gas amount (EGR), swirl level and injection pressure. Tab. 2. provides an overview of the variation range of the combustion system parameters.

Engine speed	3000 rpm
IMEP	8.3 bar
SOI	1 – 10 deg. CA BTDC
EGR	12 – 20 %
Swirl	0 – 74%
Inj. Pressure	1200 – 1600 bar

Tab. 2. Engine operating conditions and parameter variation range

For the entire set of the operating parameter variations covered by the CFD simulations, corresponding test-bed measurements are carried out in order to provide the data base for assessment of the CFD calculation results with respect to the accuracy of the predicted in-cylinder pressure traces and engine out emission data for NO and soot.

RESULTS

In the following, selected results obtained for the combustion system parameter variations are presented and discussed. Fig. 3. shows the temperature and pollutant species distribution in a section across the spray/cylinder axis at three different crank-angle positions for the baseline case. The depicted results provide a qualitative view of the major processes governing diesel combustion, i.e. the spatial and temporal flame and pollutant concentration evolution with its characteristics mainly determined by the spray injection process and its interaction with the spray induced flow motion and the piston bowl geometry.

Clearly visible is the cooling effect of the evaporating fuel spray on the in-cylinder charge prior to the onset of ignition and during the main combustion phase. The onset of auto-ignition occurs at the periphery of the fuel vapor cloud and rapidly consumes all fuel evaporated during the ignition delay

phase, leading to regions with high, near-adiabatic flame temperature. The premixed combustion then turns into a diffusion-type flame regime, with the evaporating fuel spray acting as a flame holder, stabilizing the flame around the fuel vapor plume. At the end of the injection phase, around 10 degrees crank-angle after top dead centre (10 deg. CA ATDC), the stabilizing effect of the fuel spray induced flow field ceases and the evolution of the flame and the hot combustion products gets dominated by the charge motion inside the piston bowl.

The NO formation starts-off at the locations of the initial combustion onset and in the premixed combustion zones and then continuously gets formed in the slightly fuel lean, high temperature regions. Soot is mainly formed at the fuel rich side of the diffusion flame and cumulates at the outer bowl periphery close to the walls. This is mainly due to convective effects of the spray induced flow motion and due to slow soot oxidation caused by insufficient air entrainment and the cooling effect close to the piston bowl.

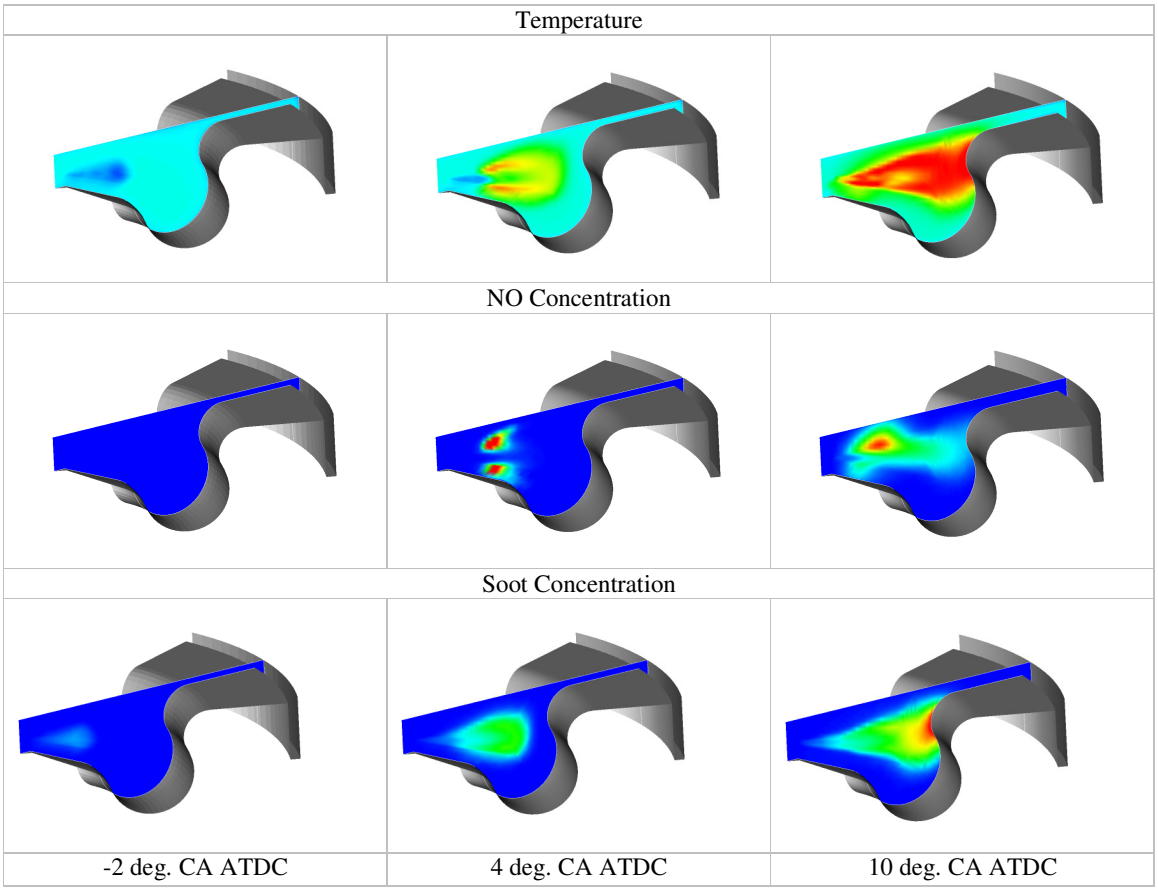

Fig. 3. Temperature, NO and soot distribution at three different crank-angle positions [5]

Besides the qualitative insight into the governing in-cylinder flow and mixture formation processes that are determining local fuel conversion and pollutant formation rates, especially the cylinder averaged quantities, such as cylinder pressure trace, rate of heat release as well as pollutant concentrations at the time of exhaust valve opening are of interest to the development engineer for assessment of engine performance and emission characteristics. Hence, the calculated cylinder pressure traces and pollutant concentration trends need to be in good agreement with the real engine behavior in order to draw sound conclusions on the impact of combustion system parameter variations on the trade-off between soot, NO and specific fuel consumption based on simulation results only.

Fig. 4. shows a comparison of measured and calculated cylinder pressure traces and heat release rates for a variation of the combustion system parameters. Following the Design of Experiment (DoE) approach adopted to select the combustion system parameter variations the cases A to D are different in terms of residual gas content, start of injection, injection pressure and swirl number. Aimed at delivering the identical indicated mean effective pressure of 8.3 bar, the resulting heat release rates and cylinder pressure traces only show subtle differences between the four displayed test cases. All heat release rates show a pronounced premixed peak, followed by a diffusion combustion phase of similar intensity and shape, with the peak firing pressure level well above the peak compression pressure level.

The calculated pressure traces are in very good agreement with the measurements for the compression, combustion and expansion phase. The good correlation between calculation and measurement during the compression phase is a clear indicator for the validity of the chosen approach for determining the CFD initial and boundary conditions. The good overall agreement of the measured and calculated cylinder pressure traces in the late phase of combustion and during the entire expansion stroke also clearly indicates that the overall energy balances and wall heat losses in the CFD calculations are in good agreement with the real engine configuration. The comparison of the calculated with the measured cylinder pressure traces during the combustion phase shows that the spray, auto-ignition and combustion models adopted in the present analysis well capture the governing physical and chemical processes.

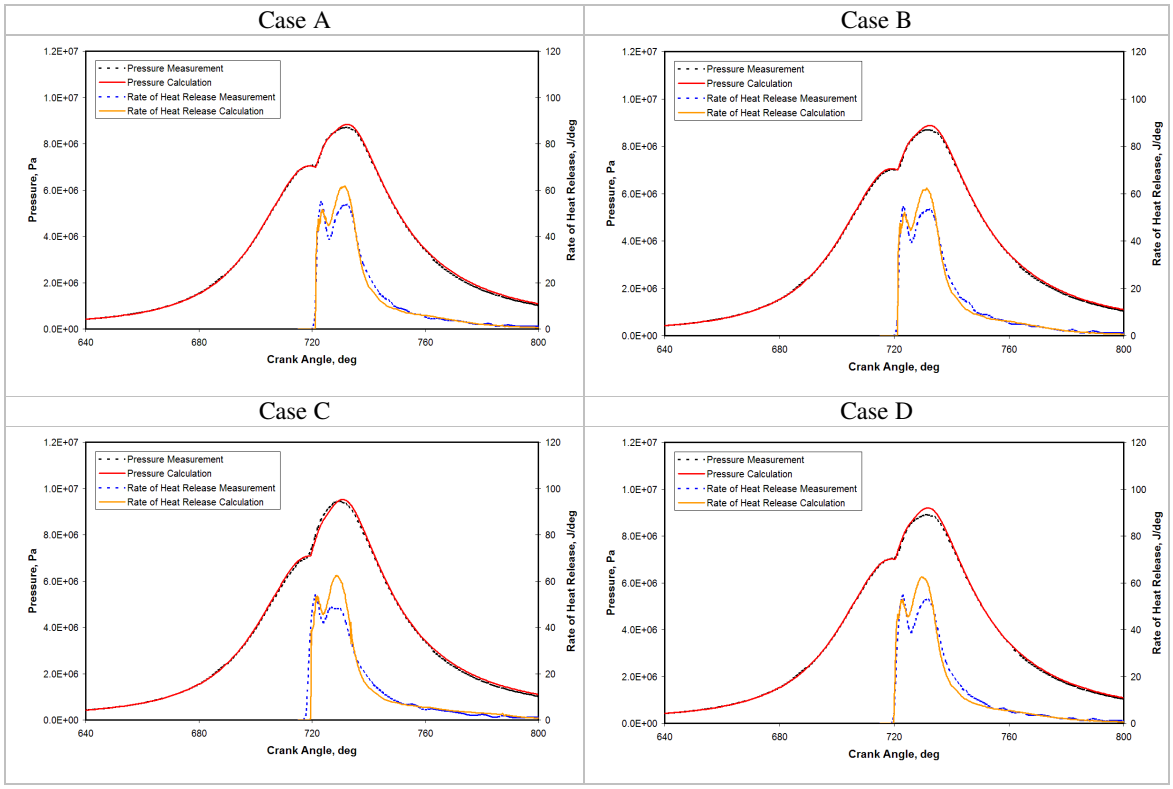

Fig. 4. Calculated and measured pressure trace and rate of heat release for selected combustion system parameter variations [19]

Although the calculated cylinder pressure traces very well match the measured ones, the heat release rates during the diffusion controlled combustion phase show some slight deviation from the "measured" ones. This can mainly be attributed to the fact that the heat release from the CFD calculations is evaluated directly from the chemical heat release in the gas phase, whereas the

"measured" heat release rate is calculated on the basis of a quasi-dimensional combustion analysis tool based on the measured in-cylinder pressure trace.

Additional results of the combustion system parameter variations are shown in Fig. 5. Here, the calculated peak firing pressure and the timing of peak firing pressure are compared to their corresponding measured values for the range of investigated parameter variations. Again, the calculated results show good overall agreement with the measured data for the conducted parameter variations by adopting identical combustion model parameter values for all cases.

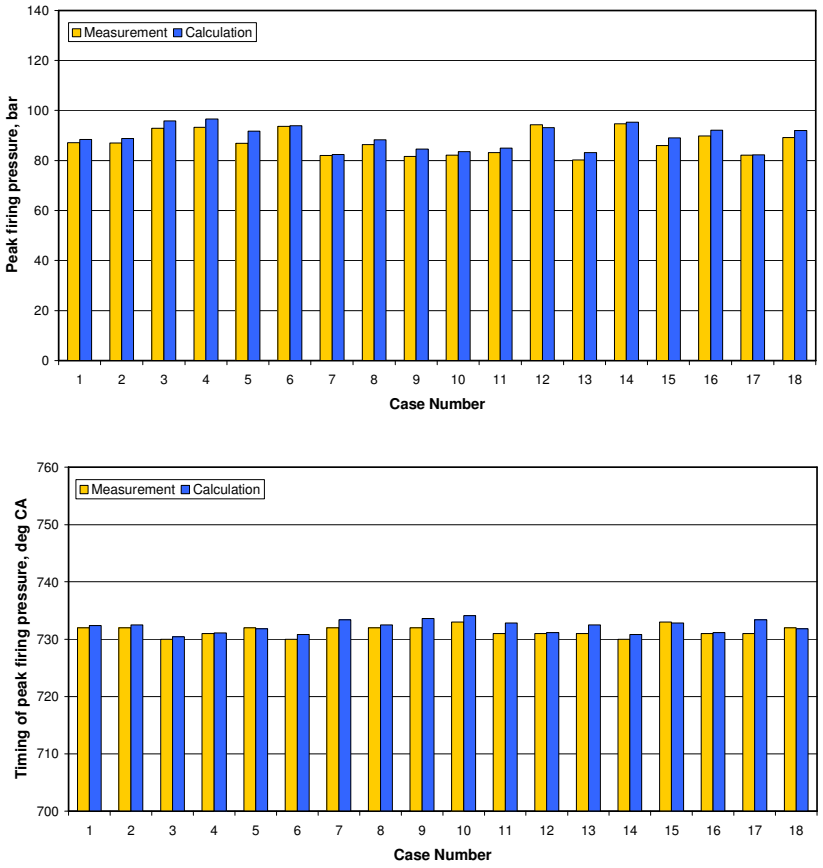

Fig. 5. Comparison of calculated and measured peak firing pressure (top) and timing of peak firing pressure (bottom) for the investigated range of combustion system parameter variations [19]

In Fig. 6. a comparison of the calculated and measured NO and soot levels is presented for the entire range of investigated combustion system parameter variations. Regarding the accuracy of the pollutant formation models adopted in the present study it can be observed from the results in Fig. 6. that the NO formation trends are well captured by the thermal/prompt NO formation model applied. Also the magnitude of concentration changes in the NO emission level is reasonably well captured for the majority of cases. Thermal NO formation is found to be the dominant mechanism for the investigated combustion system parameter variations. The soot formation trends are also reasonably well matched by the model used in the present study. Although in some cases the trends are overestimated the results provide a consistent picture of the soot formation characteristics for the investigated combustion system parameter variations.

A detailed analysis of the NO and soot formation trends displayed in Fig.6. shows that the in-cylinder NO and soot formation characteristics are considerably influenced by the combustion system

parameter variations. Regarding the NO concentrations nearly a factor of three can be observed between the minimum and maximum achievable values. Concerning soot, minimum and maximum quantities obtained with the present combustion system parameter variations differ even by a factor of up to four. Additionally, the well known NO/soot trade-off is also clearly visible for all system parameter variations performed in the present study. Out of the results displayed in Fig.6. it turns out that case number 10 provides the best improvement in the soot emission level in comparison with the reference case by showing only a small increase in engine out NO emissions – a conclusion that is confirmed by both the CFD calculations and the experimental data.

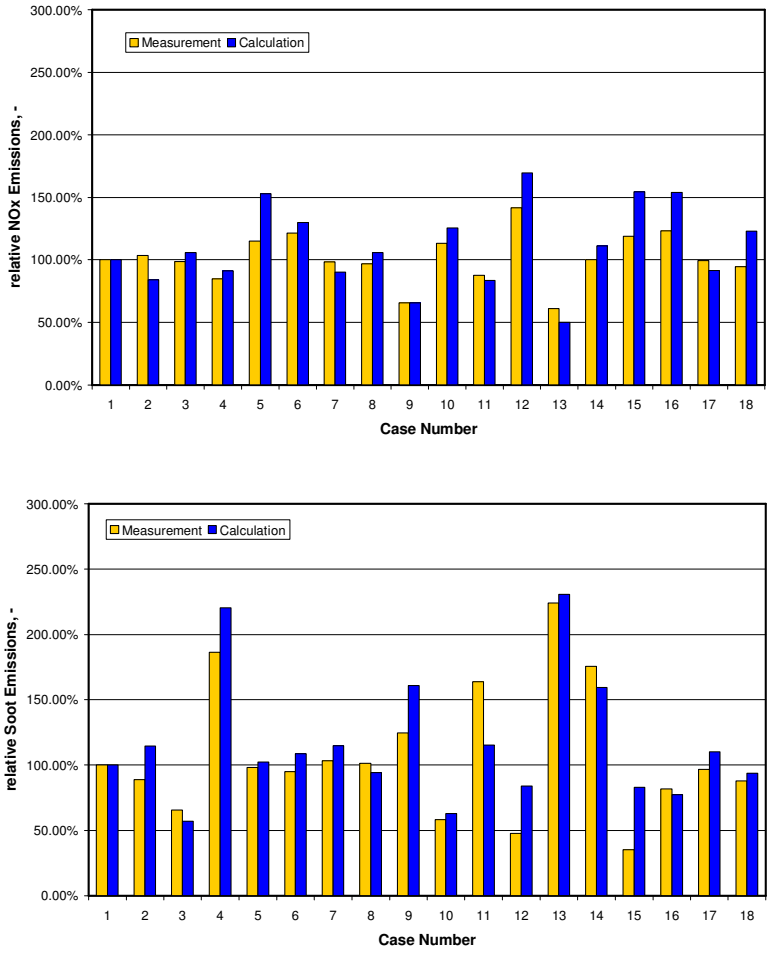

Fig. 6. Comparison of calculated and measured normalized NO (top) and soot (bottom) concentrations for the investigated range of combustion system parameter variations

SUMMARY

The impact of combustion system parameter variations on cylinder pressure, NO and soot formation characteristics is analyzed for a high-speed DI-diesel engine adopting the commercial CFD code FIRE. The parameter studies comprise of a systematic variation of rail pressure, swirl intensity, start of injection and exhaust gas return rate for a part load operating point. CFD results demonstrating the influence of the combustion system parameter variations on cylinder pressure, NO and soot formation trends are shown for a selected set of parameter variations. The CFD results clearly indicate the impact of the system parameter variations on the NO and soot emission characteristics and the ability of the adopted models to reflect the results sensitivity. Comparison of in-cylinder pressure traces, heat

release rates and pollutant formation results with the corresponding experimental data shows good agreement and confirm the validity of the adopted models as well as the overall calculation methodology used in the present work. The good agreement between the calculated and measured combustion and pollutant formation characteristics for the range of combustion system parameter variations investigated in the present study is considered to provide a sound basis for the increasing future use of CFD for analysis and optimization of DI-diesel engine combustion systems.

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