Advanced modeling of DI Diesel Engines: Investigations on Combustion, High EGR level and multiple-injection Application to DI Diesel Combustion Optimization

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The development of CFD methodology for Internal Combustion Engine represent a particular challenge because of many complex features and phenomena, perhaps more than any other widely-used mechanical device.

Understand the processes taking place in the combustion chamber and the correlation between parameters and therefore a way to support the design is today essential to explore new solutions, reduce the cost and improve the development efficiency.

The aim of the present paper is to describe the recent development of the general multi-purpose code STAR-CD in the field of Internal Combustion Modeling with a special emphasis on DI Diesel Engines operating with very high level of Exhaust Gases Recirculation (Higher than 30%) and using multiple-injection strategy.

An enhancement of the new combustion model developed in the GSM (Groupement Scientifique Moteurs including IFP, PSA and RENAULT) and implemented in STAR-CD, The Extended Coherent Flame Model-3Z (ECFM-3Z) is described first. This model enable to compute combustion for operating conditions with large EGR amount in DI Diesel engines has been completed.

Predictions have been compared with extensive data from a DI Diesel Engine in production over a wide range of operating conditions. The results show that the combustion model used in combination with a two steps auto-ignition model gives realistic Heat Release History as well as emission prediction.

In addition, the combination of the CFD tool with a multi-objective optimization tool ModeFrontier^{TM} is applied to optimize the operating conditions as well as the piston bowl shape design for a DI Diesel engine for the fuel consumption, emissions (Soot and NOx) and noise reduction.

1.0 INTRODUCTION

The development of CFD methodology for IC engine design represents a particular challenge due to the complex physics and mechanics, perhaps more than with any other widely-used mechanical device [1]. Improved understanding is essential to explore new solutions, reduce costs, and improve development efficiency. Although substantial advances have been made in all areas (turbulence, spray modeling, combustion, numerical methods, parallel computing, pre- and post-processing, etc.), there are numerous additional requirements to be met for it to become a design tool. The aim of this paper is to describe the recent developments in the multi-purpose CFD code STAR-CD [2] in the field of IC engine modeling with a special emphasis on DI Diesel engine combustion. An enhanced spray model and a new combustion model for GDI and Diesel engines is presented along with the optimization of a light duty DI Diesel engine using STAR-CD and the multi-objectives optimization tool ModeFrontier^{TM}.

2.0 THE MATHEMATICAL MODELS

2.1 THE SPRAY MODELS

The modeling of fuel injection processes is an essential part of DI Diesel engine simulation. The existing fully coupled stochastic Lagrangian-Eulerian approach used in STAR-CD [2] has been enhanced to avoid the necessity to empirically tune coefficients or other inputs of the spray model. These issues have been addressed in various ways in the enhanced implementation of the nozzle, atomization, and collision models.

2.1.1 The Nozzle Flow Model

The injection velocity, i.e. the velocity of the liquid fuel as it exits the nozzle and enters the combustion chamber, is one the most important parameters in a spray calculation. It strongly influences the atomization and break-up processes, the spray penetration, the inter-phase transfer processes, and the droplet-droplet interaction. The main feature of this model is the recognition of the creation of a separation/cavitation region emanating from the nozzle hole entrance. This results in the reduction of the exit cross-sectional area below its geometric value, which in turn increases the injection velocity. Depending on the pressure in the chamber relative to the critical pressure at which cavitation commences, and the length of the cavitation region, the model distinguishes three different flow regimes, i.e. the non-cavitating flow, the cavitating flow inside the nozzle, and the cavitating flow at the nozzle exit.

2.1.2 The Atomization Model

From the various built-in atomization models in STAR-CD, Huh’s [3] atomization model was chosen for this study. The characteristics and assumptions of this model are presented here. Huh’s model asserts that the two most important mechanisms in spray atomization are the gas inertia and the internal turbulence stresses generated in the nozzle. A conceptual picture can be described in two stages:

1. The turbulence generated in the nozzle hole produces initial perturbations on the jet surface when it exits the hole.
2. Once the perturbations have reached a certain level, they grow exponentially via pressure forces induced through interaction with the surrounding gas, until these perturbations become detached from the jet surface as droplets.

The model estimates the initial perturbations from an analysis of the flow through the hole and then uses established wave growth theory to represent the atomization process. The perturbation amplitude obeys a dispersion equation as derived by Taylor. The break-up rate of the produced parent droplets (obtained from the nozzle model) is calculated as a function of an atomization time scale and an atomization length scale. The diameter of secondary droplets formed from parent droplet break-up is estimated from a PDF. The minimum droplet size is calculated from Kelvin-Helmoltz instability theory. The atomization length and time scales are used to calculate the spray semi-cone angle. Finally, the estimation of initial velocity for each droplet is based on the assumption of equal probability of velocity direction within the spray cone.

2. THE COMBUSTION MODEL: ECFM-3Z

The ECFM-3Z model is a combustion model based on a flame surface density transport equation and a mixing model that can describe inhomogeneous turbulent premixed and diffusion combustion. This model is an extension of the ECFM [4] combustion model, previously implemented in STAR-CD and extensively validated for GDI applications. The idea is to divide the computational domain taking into account the local stratification. In the mixed zone, standard ECFM is computed, with an improved version of the post-flame chemistry model in the burned gases and an auto-ignition model in the unburned gases. The evolution of the mass included in the 3 mixing zones (Figure 1) are computed and modified with the help of a mixing model.

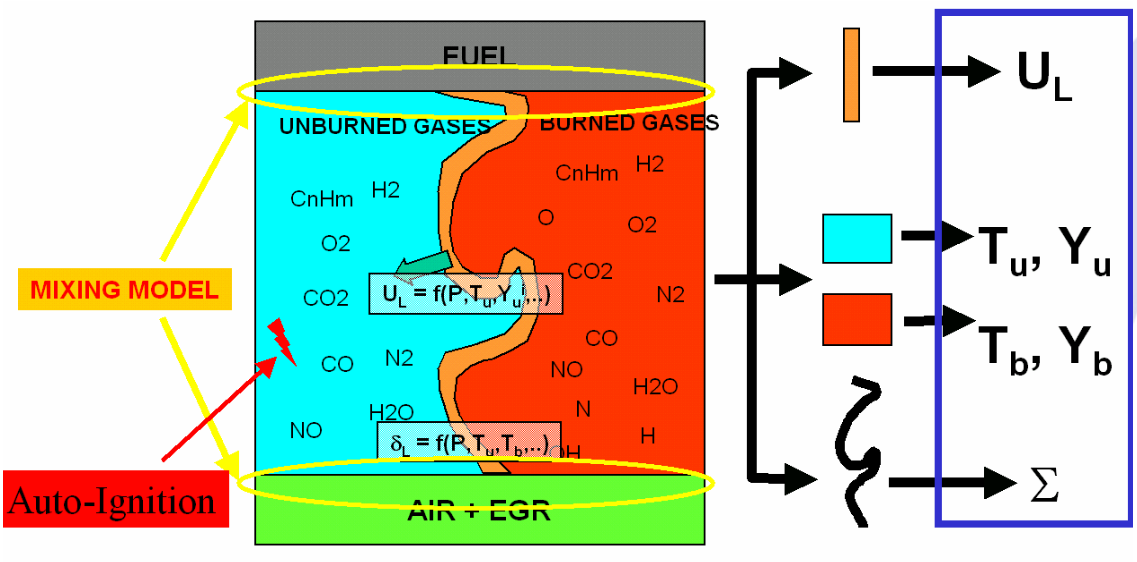


Figure 1: Principle of the ECFM-3Z model

2.2.1 The Auto-Ignition Model

For new low emissions combustion concepts such as HCCI engines or DI Diesel Engines wit pilot-injection, cool flames may occur. The main auto-ignition delay is strongly dependant on thermodynamic conditions (temperature and pressure). Therefore the heat release observed during the cool flame will affect the global auto-ignition delay. Base on this conclusion, a new double delay auto-ignition model, based on tabulated temperature profiles issued from complex chemistry, is proposed as illustrated in figure 2.

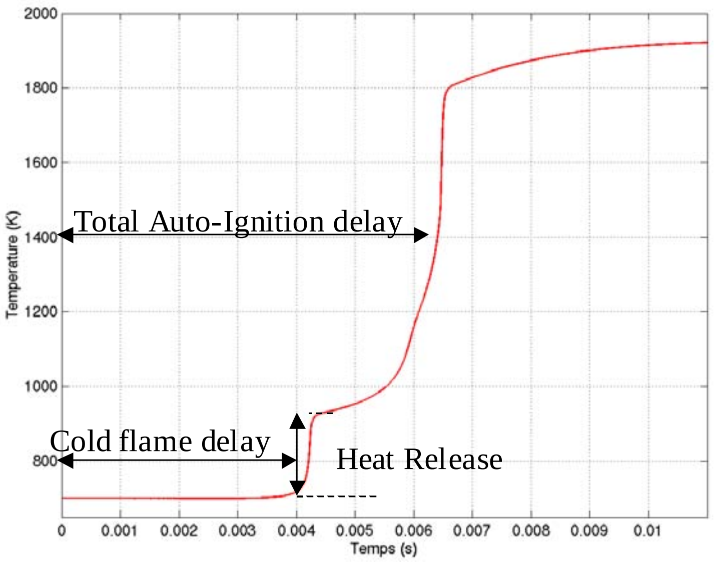


Figure 2: Temperature profile during auto-ignition from complex chemistry calculation

2.2.2 The Regression Model

In order to be able to compute multi injection , multi cycles or local extinction, a simplified regression model has been introduced. This model just transfers burned gas quantities into unburned gas quantities when the local burned gas temperature is too low. This model

2.2.3 The Mixing Model

The first version of the mixing model is rather simple, based on the exchange with mean quantities. The amount of mixing is computed with a characteristic time scale based on the k-epsilon model. In this model we compute the evolution of two quantities: the unmixed fuel and the unmixed oxygen.

2.2.4 The Post-Flame Chemistry

The post-flame chemistry of the model is an improved version of the post-flame chemistry of the ECFM model. The major changes are the addition of a soot model and the introduction of kinetic oxidation of CO. The considered equilibrium reactions are:

$$\mathbf{N_2 \leftrightarrow 2N}$$
$$\mathbf{O_2 \leftrightarrow 2O}$$
$$\mathbf{H_2 \leftrightarrow 2H}$$
$$\mathbf{2\,OH \leftrightarrow O_2 + H_2}$$
$$\mathbf{2\,H_2O \leftrightarrow O_2 + 2H_2}$$

For the kinetic oxidation of CO we have:

$$\mathbf{CO + OH \leftrightarrow CO_2 + H}$$

NO is calculated using the Extended Zeldovich mechanism.

2.2.5 The Soot Model

The Wisconsin ERC Soot Model is used for this first version considering a competing formation rate and an oxidation rate.

3.0 DI DIESEL COMBUSTION: MODEL VERIFICATION

ENGINE A: This is a typical light duty Diesel engine with displacement of 1.0 liter/cylinder equipped with a six-hole injector. The piston bowl shape is a Mexican hat profile with an open chamber. The swirl level is moderate and pilot injection is considered
ENGINE B: This is also a typical light duty Diesel engine with a displacement of 1.80 liter/cylinder equipped with an eight-hole injector. The piston bowl is a re-entrant bowl type.

3.1 GLOBAL CYLINDER DATA

Several cases were computed for both engines and global quantities were compared to experimental data.

A comparison between computed and measured in-cylinder pressure is presented in Figure 2 and Figure 3 in order to assess the accuracy of the computational model with respect to the prediction of global cycle averaged cylinder quantities. In addition, the derivative of the in-cylinder pressure is compared to experiment for noise purposes (Figure 4). It can be seen that the pressure gradient magnitude is quite well predicted as well as its location in the cycle.

3.2 EMISSIONS

The calculated global quantities of pollutant data serve as the basis for further assessment of the spray and combustion models' behavior under engine operating condition parameter variations. This enables the study of the influence of injection timing, %EGR, etc. on soot and NOx formation. Figure 5 shows representative results of the relative soot and NOx formation trends for different %EGR levels.

3.3 HEAT RELEASE

From the STAR-CD runs, the rate of heat release is directly extracted from the reactive species and their respective heat of formation.
The name of experimental heat release is in reality another interpretation of the experimental measured in-cylinder pressure (and its derivative) through the first principle of thermodynamic and the equation of state.

Precautions have to be taken when one would like to compare these two quantities. The first one was shown in figure 4 in which one could see a typical comparison between measured and computed pressure derivative.

Therefore one can adjust the thermodynamic model calculating the heat release from the experimental pressure and can compare it to the STAR-CD predictions. This is shown in figure 7. The comparison shows a quite good agreement.

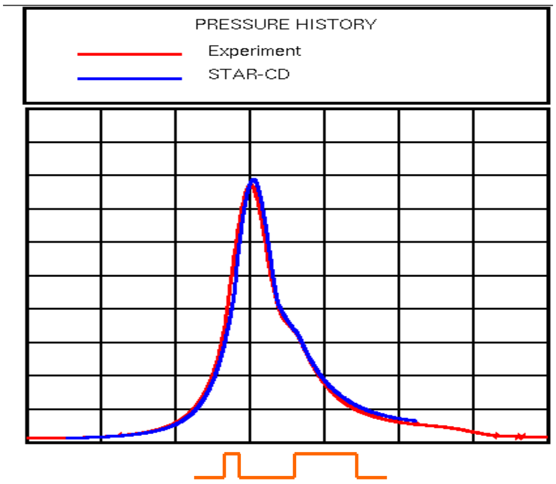


Figure 2: Comparison between calculated and measured cylinder pressure: Engine A, 50% Load, 2000 RPM

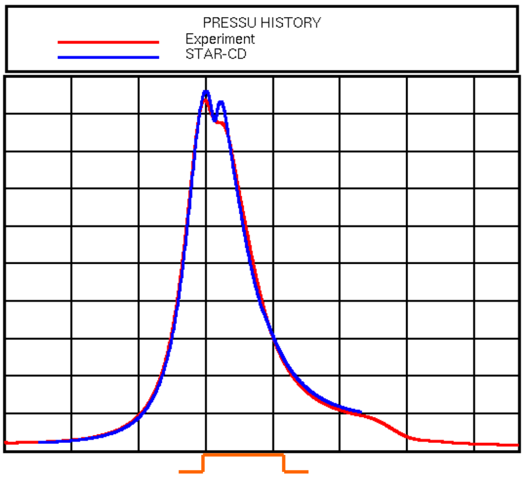


Figure 3: Comparison between calculated and measured cylinder pressure: Engine B, 100% Load, 1200 RPM

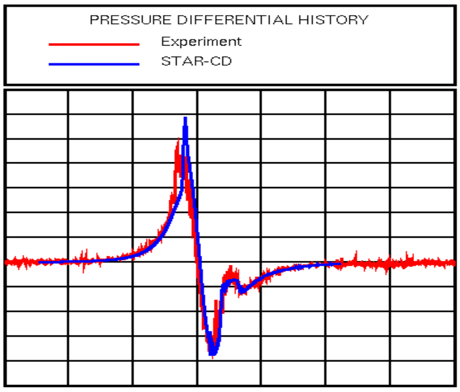


Figure 4: Pressure gradient history

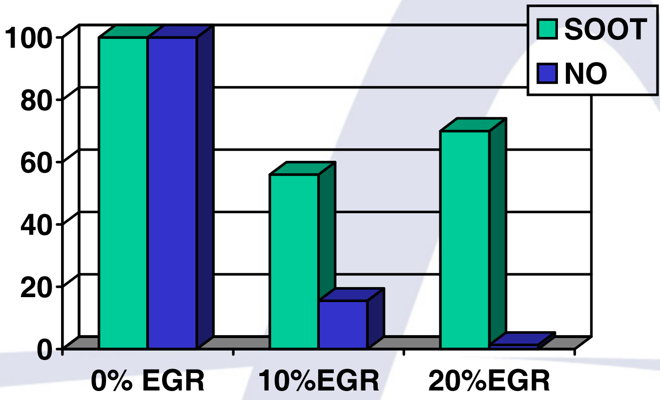
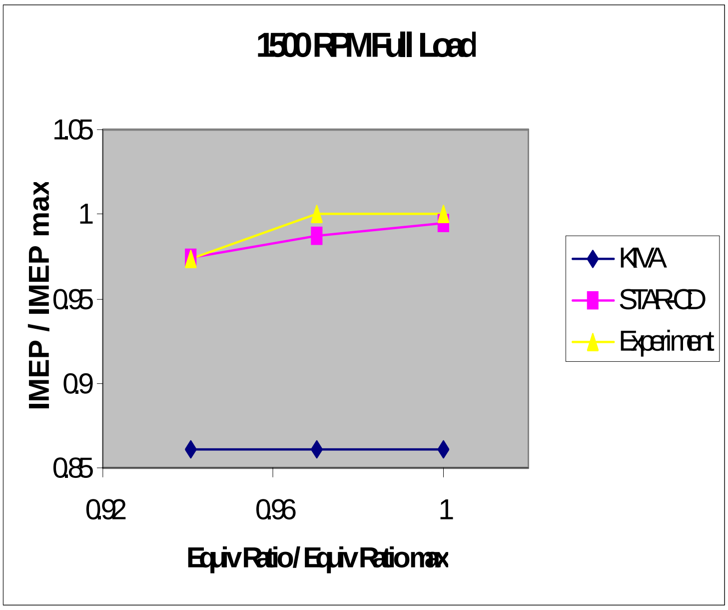


Figure 5: Relative soot and NO formation trends at Different % EGR levels



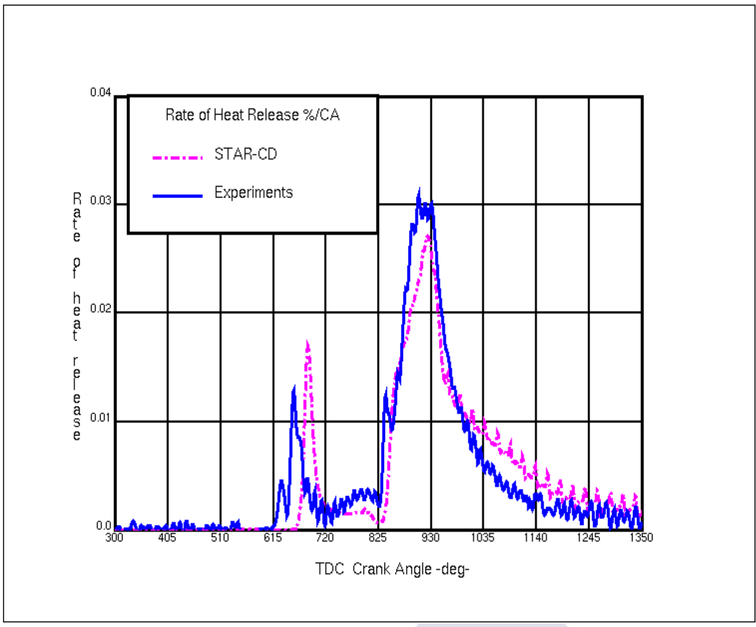
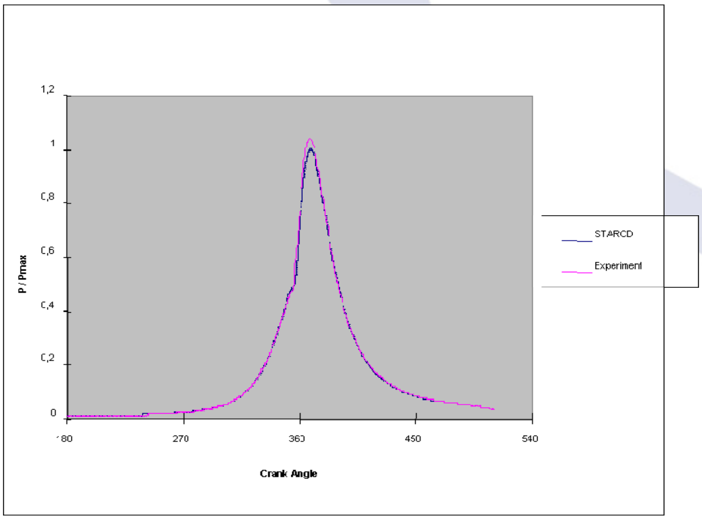


Figure 6 : Calculated and measured IMEP

Figure 7 : Rate of Heat Release

3.4 Full load Operating condition

Two different engine speeds were computed for this engine and global quantities were compared to experimental data. A comparison between computed and measured in-cylinder pressure is presented in Figures 8 and 9, in order to assess the accuracy of the computational model with respect to the prediction of global cycle averaged cylinder quantities. Another interesting model verification is took at the IMEP and the trends obtained when the varying the global equivalence ratio for soot limit investigation. A typical result is presented in figure 6. As it is shown, the predicted results show a very good agreement with measured values, which a good indication for good prediction in wall heat transfers as well.



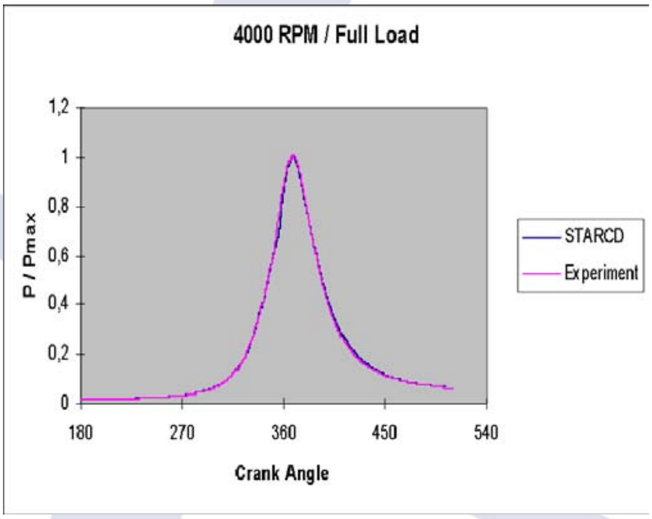


Figure 8: Comparison between calculated and measured in-cylinder pressure: 100% load, 1500 rpm

Figure 9: Comparison between calculated and measured in-cylinder pressure: 100% load, 4000 rpm

3.5 Part load Operating condition

It is well known that increasing the EGR level is a good solution for reducing NOx emissions in DI Diesel engines. However, compromise between NOx emissions and the other important pollutant, which is the soot, is also well known. Pilot-injection (or Post-injection) is then used to decrease the soot level.

The calculated global quantities of pollutant data serve as the basis for further assessment of the spray and combustion models behavior under engine operating condition parameter variations. This enables the study of the influence of injection timing, %EGR, etc on soot and NOx formation for four different operating conditions. (C.f. Table 1).

	RPM	Injector	Pilot injection	Load (%)	EGR (%)
OP 1	1500	Injector 1	Yes	20	40
OP 2	2000	Injector 1	Yes	40	10
OP 3	1500	Injector 2	Yes	20	40
OP 4	2000	Injector 2	No	40	10

Table 1: Part load Operating conditions

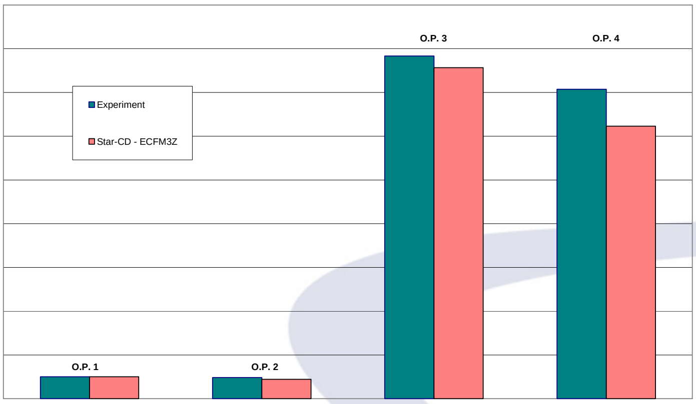


Figure 10: Comparison of NOx at EVO – Normalized Results based on OP1

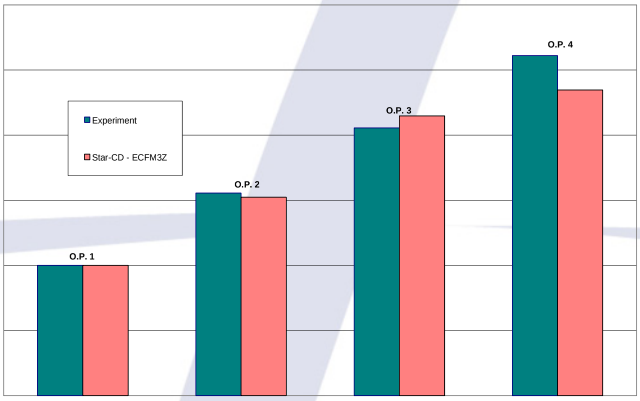


Figure 11: Comparison of Soot at EVO – Normalized Results based on OP1

Figure 10 and 11 show also results at EVO of relative soot and NOx formation trends obtained for this engine for the four different operating conditions. One can observe that trends are very well predicted.

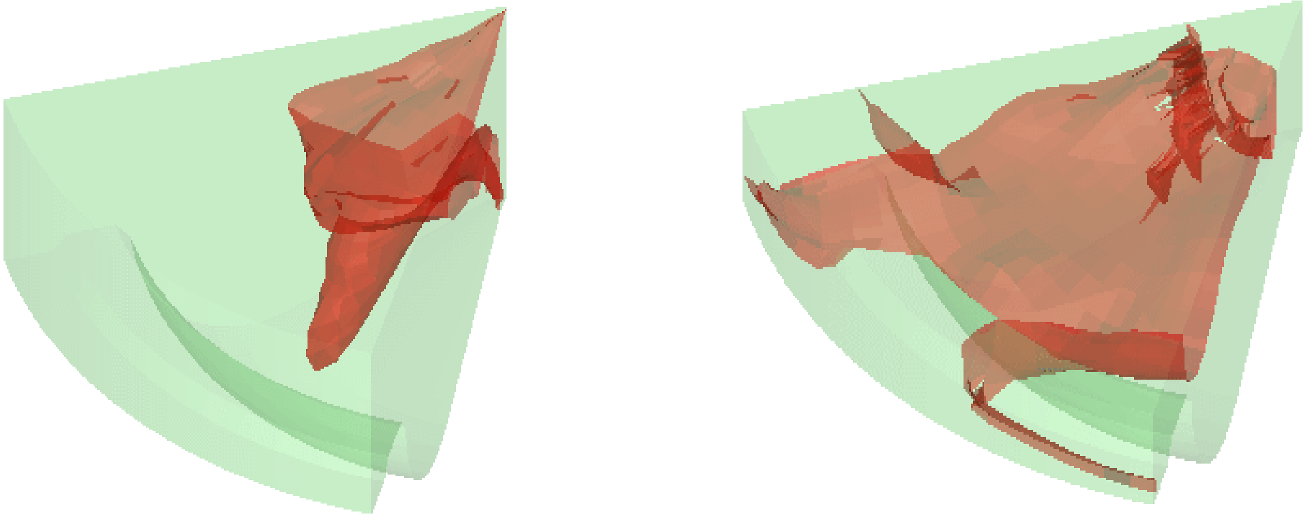
4.0 HCCI COMBUSTION

Operating an engine in Homogeneous Charge Compression Ignition (HCCI) mode requires a homogeneous mixture of air, fuel and residual gases. The mixture in then burnt by Controlled Auto-Ignition (CAI) in an ideal case.

Therefore, a good mixing model and detailed fuel chemistry is needed. The ECFM-3Z contains all appropriate sub-models as described above. For this first application we have used a very simple scheme for chemistry based on experimental correlation based on Ignition Delay measurements.

This was applied to a Diesel HCCI mode. In Figure 12 are plotted the iso-surfaces where Auto-Ignition can occurs and compare a Diesel Mode with a Diesel HCCI mode. This is very important information showing clearly that the mixture is not completed in the Diesel HCCI mode.

This is also illustrated by the rate of heat release in figure 13 showing a large diffusion phase occurring after TDC.



Diesel mode Diesel HCCI Mode

Figure 12 : Iso-surface for Auto-Ignition Sites

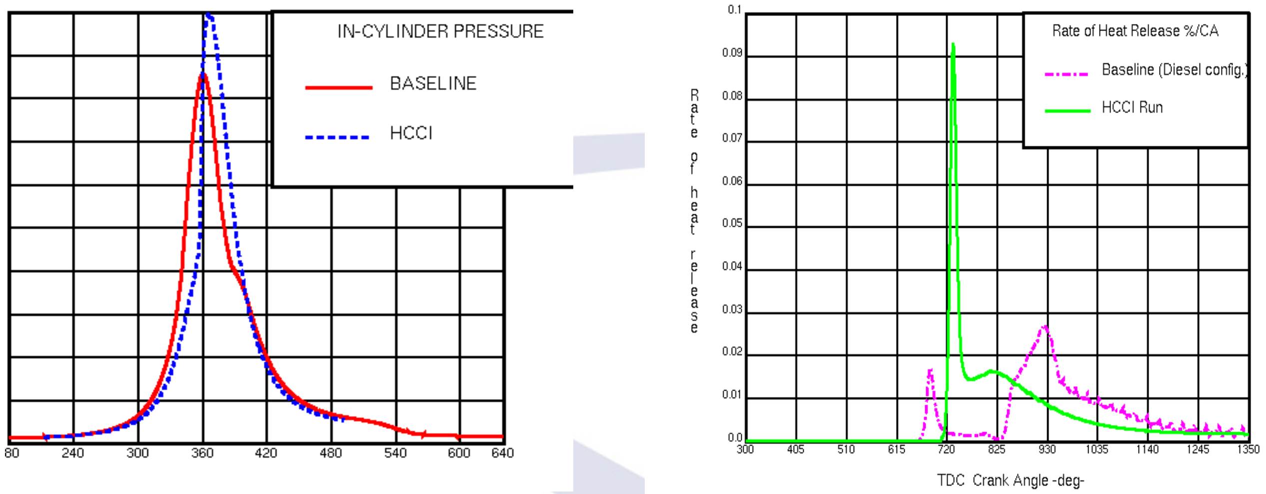


Figure 13 : In-Cylinder pressure and Rate Of Heat Release

4.0 DI DIESEL COMBUSTION: OPTIMIZATION

DI Diesel engine combustion chamber design (piston bowl shape, aspect ratio, etc.), fuel calibration, swirl, %EGR levels, etc., represent important independent parameters to optimize in order to meet the increasing demands of reduced fuel consumption and reduced emissions production. Even using a good optimization tool combined with test bench experiments is not sufficient, because the optimizer requires an instantaneous interaction between its algorithm and the new design configuration. This means: Stop the measurements. Apply the new design. Measure again. This is very time consuming and costly. Therefore, it is a good opportunity for CFD combined with an optimization tool to optimize and better understand DI Diesel combustion.

As an example, Figure 14 and Table 2 show the five different independent parameters used to obtain the optimum configuration that minimizes the soot and NOx levels and maximize the piston work. These parameters are the swirl level (SWIRL), %EGR level (%EGR), the number of injector holes (N_holes), the injection timing for the main injection (Tis), and the time between the end of the pilot injection and the start of the main injection (Dpi)

The simulation was conducted on a sector mesh and therefore, the angle of the sector was a function of the number of injector holes as well as the nozzle diameter. The injection pressure was maintained constant (the rail pressure). Table 1 summarizes the desired range of variation for the independent parameters as well as their respective increments.

The purpose of an optimization tool is to find the optimum configuration with a minimum number of calculations, i.e. reduce the cost and effort.

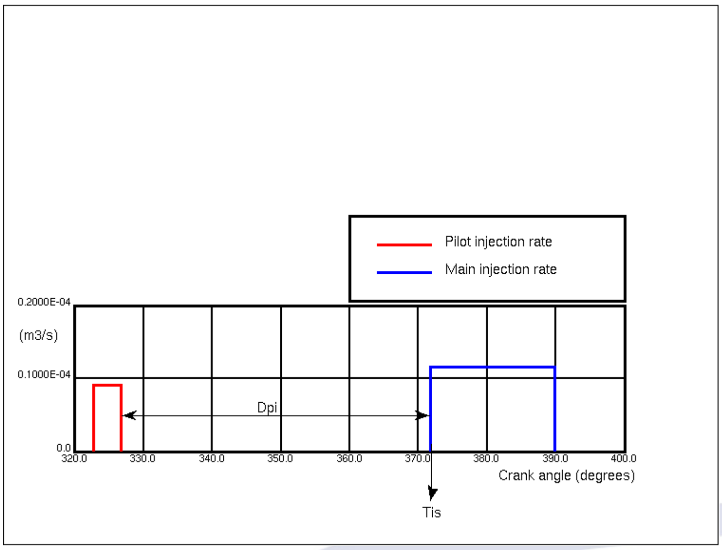


Figure 14 : Injection profile

	Lower	Upper	Increment
SWIRL	0.3	2.3	0.2 (11)
%EGR	0	20	4 (6)
N_holes	6	12	2 (4)
TIS (CA)	350	380	2 (16)
DPI (CA)	10	50	5 (9)

Table 2: Independent parameters - range and increments

ModeFrontier TM was chosen as the optimization program. For the five independent parameters listed above, STAR-CD calculates the soot and NOx levels and the piston work during the closed phase of the engine cycle.

Thanks to the input parameter flexibility of es-ice and PROSTAR, the pre and post-processor of STAR-CD, it is possible to easily achieve such a process flow with ModeFrontier including parameters affecting the geometry. The SOBOL algorithm in ModeFrontier is chosen to determine the original population. We limited ourselves here to only 10 runs. Then the MOGA (Multi Objective Genetic Algorithm) is chosen for the optimization process.

One can see clearly that after the first 10 runs (design chosen randomly), the procedure is trying to minimize soot and NO and optimize the piston work. The result after 25 runs is summarized in Figure 15 and Table 3.

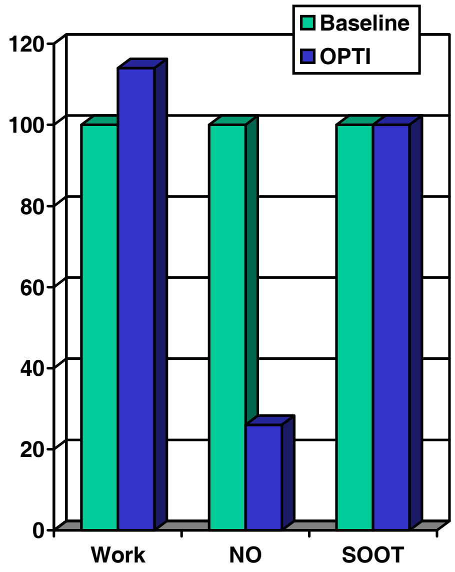


Figure 15: Optimization results after 25 runs

OPERATING CONDITIONS	**Baseline**	**Optimized**
Swirl Level	**1.0**	**1.86**
%EGR	**0.0**	**12.0**
Injection Timing Main (ATDC)	**12.0**	**-6.0**
End of Pilot Injection – Start of Main	**40**	**20**
Number of Injector Holes	**N**	**ident**

Table 3: Summary of optimized analysis parameters

In the process of optimization, it appeared that the soot is not reduced and probably one needs to execute more, or introduce another independent parameter like the injection pressure. However, because of the piston work increase, one can consider that the optimization is achieved just by reducing the amount of injected fuel.

5.0 CONCLUSIONS

Presented in this paper are a new combustion model, the ECFM-3Z model, based on a flame surface density transport equation and a mixing model that can describe inhomogeneous turbulent premixed and diffusion combustion and substantial improvements of the spray model in STAR-CD. The combustion model is coupled with improved burned gas chemistry that allows CO, soot, and NOx formation calculations. After validating the model with several engine configurations and operating conditions, a method of optimizing DI Diesel combustion was presented in conjunction with an optimization tool.

6.0 REFRENCES

[1] Gosman, A.D. “State of the art of multi-dimensional modeling of engine reacting flows.” **Oil & Gas Science Technology, Vol. 54 (1999)**

[2] STAR-CD V3.15 PROSTAR & es-ice are Trademarks of CD-adapco Group

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