

# Three-Dimensional Modeling of Combustion Process, Soot and NO<sub>x</sub> formation In a Direct-injection Diesel Engine

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## Abstract

This paper is presented to study the combustion process and emissions in a direct injection diesel engine. Computations are carried out using a three-dimensional model for flows, sprays, combustion and emissions in Diesel engines. Interactions between combustion and emissions with flow field are considered and it is shown that soot mass fraction increases at regions with low turbulence intensity and fuel rich zones. Impingement of spray with the piston walls is also modeled by Wall-jet functions and is shown that soot mass fraction tends to increase at impinging zones. Also in high temperature areas where Air Fuel Ratio (AFR) nears unity and oxygen is available, NO<sub>x</sub> mass fraction will increase. Results of this model show a good agreement with the corresponding data in the literature.

**Keywords: Diesel Engine, Turbulence, Combustion, Spray, Emission**

## 1. Introduction

■ In a very competitive world improvement of engine performance has become an important issue for automotive manufacturers. In order to improve the engine performance the combustion process is now being studied in more detail. Also, the recent global environmental regulations for reducing engine emissions have forced engine designers to explore new engine concepts and to study the effect of engine parameters on the formation of pollutant emissions. Simulation of the

combustion system by means of computer modeling makes it possible to explore combustion regimes that may be difficult and/or expensive to achieve with experiments [1].

Such modeling first started in 1950 with simple thermodynamic models for engine cycles which then were extended in 1970 to multi-zone models. Nowadays with the progressive development of computational fluid dynamics (CFD) and flow field models, it is also possible to study and predict droplet distribution, temperature, pressure and other parameters at every desired point and time within the combustion chamber.

Flow field models, such as KIVA II code in 1990 [2, 3] and numerical Ricardo Code which was employed to investigate an optimum value for gas fuel injector angle in a dual fuel diesel-gas engine to obtain minimum UHC emissions in 1992 [4], are

premiere examples. Choi Wook, et al [5] has used STARCD code and PIV analysis to study In-cylinder flow field of a single cylinder DI diesel engine. It was indicated that high Reynolds k-ε turbulent model pretty much satisfies such flow fields.

The research group of Prof. Reitz at University of Wisconsin-Madison performed modeling the combustion in a quiescent chamber engine, in order to evaluate the NO<sub>x</sub> particulate trade off, varying the injection timing, the injection pressure and the split injection dwell angle. They used an improved KIVA II version, adopting the Hiroyasu expression for soot formation and the Nagle et al Mechanism for soot oxidation [6].

The three-dimensional model for flow, spray and combustion is based on FIRE code to predict and study the combustion process and emissions formation in OM-355 diesel engine.

## 2. Model specification

The numerical model for heavy duty OM-355 diesel engine with the specifications on table 1 is based on Fire CFD code [7]. Engine speed of 1400 rpm is selected which produces highest emissions trade off. Fuel injection pressure is assumed constant during injection and set to 195 bar and the injection period starts from -18 °CA up to 0 °CA. Calculations are carried out on the closed system from IVC at -118 °CA to EVO at 120 °CA. The centric injector has four holes and is fixed beneath cylinder head and fuel is injected at a constant rate. Ambient temperature and pressure are chosen as initial conditions. Swirl ratio is set at 1.1 for an approximately quiescent condition and considering the symmetry of the model, solution domain only covers a 90 degrees section. Fig. 1 shows the numerical grid.

Combustion process is modeled by Eddy Breakup model which is a turbulent controlled combustion model. Spray droplet breakup and distribution is modeled by advanced Wave Standard in which initial droplets have the diameter of nozzle orifice. NO<sub>x</sub> formation is modeled by the Zeldovich mechanism and Soot is modeled by the Kennedy, Hiroyasu and Magnussen mechanism.

Equations used by numerical model are as follows [7]:

### 2.1 Continuum equation:

$$\frac{\partial \hat{\rho}}{\partial t} = -\frac{\partial}{\partial x_j} (\hat{\rho} \hat{U}_j) \quad (1)$$

### 2.2 k-ε Turbulent and momentum equation:

$$\rho \frac{\partial k}{\partial t} + \rho U_j \frac{\partial k}{\partial x_j} = P + G - \varepsilon + \frac{\partial}{\partial x_j} \left( \mu + \frac{\mu_t}{\sigma_k} \frac{\partial k}{\partial x_j} \right) \quad (2)$$

$$\rho \frac{D\varepsilon}{Dt} = \left( C_{\varepsilon 1} P + C_{\varepsilon 3} G + C_{\varepsilon 4} k \frac{\partial U_k}{\partial x_k} - C_{\varepsilon 2} \varepsilon \right) \frac{\varepsilon}{k} \quad (3)$$

$$+ \frac{\partial}{\partial x_j} \left( \frac{\mu_t}{\sigma_\varepsilon} \frac{\partial \varepsilon}{\partial x_j} \right)$$

$$\mu_t = C_\mu \rho \frac{k^2}{\varepsilon} \quad (4)$$

$$G = -\frac{\mu_t}{\rho \sigma_\rho} \nabla \rho \quad (5)$$

$$P = -2\mu_t S : S - \frac{2}{3} [\mu_t (trS) + K] (trS) \quad (6)$$

where

C <sub>μ</sub>	C <sub>ε1</sub>	C <sub>ε2</sub>	C <sub>ε3</sub>	C <sub>ε4</sub>	σ <sub>k</sub>	σ <sub>ε</sub>	σ <sub>ρ</sub>
0.09	1.44	1.92	0.8	0.33	1	1.3	0.9

## 3. Energy equation:

$$\rho \frac{DH}{Dt} = \rho \left( \frac{\partial H}{\partial t} + U_j \frac{\partial H}{\partial x_j} \right) \quad (7)$$

$$= \rho \dot{q}_g + \frac{\partial P}{\partial t} + \frac{\partial}{\partial x_i} (U_j \tau_{ij}) + \frac{\partial}{\partial x_j} \left( \lambda \frac{\partial T}{\partial x_j} \right)$$

## 4. Combustion rate equation (combustion model)

This model assumes that in premixed turbulent flames, the reactants (fuel and oxygen) are contained in the same eddies and are separated from eddies containing hot combustion products. The rate of dissipation of these eddies determines the rate of combustion.

$$\overline{\rho \dot{r}_{fu}} = \frac{C_{fu}}{\tau_R} \bar{\rho} \min \left( \bar{y}_{fu}, \frac{\bar{y}_{ox}}{S}, \frac{C_{pr} \bar{y}_{pr}}{1+S} \right) \quad (8)$$

The first two terms of the “minimum value of” operator determine whether fuel or oxygen is present in limiting quantity, and the third term is a reaction probability which ensures that the flame is not spread in the absence of hot products. Above equation includes three constant coefficients (C<sub>fu</sub>, τ<sub>R</sub>, C<sub>pr</sub>) in which C<sub>fu</sub> varies from 3 to 25 in diesel engines. An optimum amount was selected according to experimental data.

## 5. Spray model:

Wave breakup model is used which is further modified to account for spray wall impingement effects, and is also improved by considering droplet distortion to obtain dynamically varying drop drag coefficients [1]. The initial fuel droplets have the diameter of nozzle hole which is technically called blob injection.

Droplet dissipation rate is modeled by the following equation:

$$\tau = \frac{3.726 C_2 r}{\Lambda \Omega} \quad (9)$$

In which  $\Lambda$  and  $\Omega$  are wave length and wave growth rate and are functions of droplet characteristics and critical Weber number. Also droplet radius is assumed to obey the equation at steady state. Detailed information can be found in reference [8 and 9].

$$r_{stable} = \min \left\{ \left( \frac{3\pi^2 U}{2\Omega} \right)^{0.33}, \left( \frac{3r^2 \Lambda}{4} \right)^{0.33} \right\} \quad (10)$$

## 6. Emission models

The thermal  $\text{NO}_x$  formation mechanism is expressed in terms of the extended Zeldovich mechanism:



The Hiroyasu and Magnussen [7] mechanism for soot formation rate is modeled as the difference between soot formation and soot oxidation:

$$\frac{dm_{soot}}{dt} = \frac{dm_{form}}{dt} - \frac{dm_{oxid}}{dt} \quad (14)$$

Where

$$\frac{dm_{form}}{dt} = A_f m_{fv} p^{0.5} \exp\left(-\frac{E_a}{RT}\right) \quad (15)$$

$$\frac{dm_{oxid}}{dt} = \frac{6M_c}{\rho_s d_s} m_s R_{tot} \quad (16)$$

All above equations are taken into account simultaneously to predict spray distribution and combustion progress in the turbulent flow field, wall impingement and diesel combustion rate using two stage pressure correction algorithms.

## 7. Results and discussion

Results for combustion parameters and emissions are presented as figures or contours. To be able to address the effects of spray impingement on local emission formation, wall-jet1 wall function was employed in the model. Fig. 2 shows the predicted jet impinging, droplet distribution and fuel vapor contour at 355 °CA. Due to low swirl ratio at the heavy duty diesel engine, fuel spray interaction with piston wall seems rather probable at such low engine speeds. Fig. 3 shows the comparison between computed and measured in cylinder pressure. It can be seen that the model predictions agree well with experimental data [10]. Figs. 4 and 5 also compare the calculated and experimental results for  $\text{NO}_x$  and soot emissions respectively [7]. Fig. 6 shows mean in cylinder temperature change as a function of crank angle. Combustion process is started approximately at 360 °CA and thus followed by a great change in both pressure and temperature curves (Figs. 3 and 6). Figs. 7 and 8 show soot and  $\text{NO}_x$  mass fractions. It is seen that soot formed at early stages of combustion is oxidized up to EVO point.  $\text{NO}_x$  formation starts at about 365 °CA and continues to increase at high rate to freeze at 410 °CA.

Fig. 9 is the view of temperature contours during the combustion process in both horizontal and vertical sections from 300 °CA to 478 °CA. Iso-temperature lines are shown on the contours to verify high temperature regions. Combustion process starts about 356 °CA (Figs. 6 and 9) and temperature increases at bowl corners due to intensified turbulent flow field and oxygen availability. In Figs. 10 - 12 a general comparison is presented to verify the interactions of emissions with oxygen availability, Air Fuel Ratio (AFR) and flow field velocity for crank angles of interest during combustion.

It can be seen that with both oxygen availability and high temperature conditions satisfied  $\text{NO}_x$  formation increases, while soot concentration increases at low turbulence and velocity regions specially at impinging zones. The maximum concentration of soot is observed in regions where AFR contours indicate rich mixtures. It is also seen that  $\text{NO}_x$  concentration tends to increase in regions with AFR value near to unity.

Also, the opposing nature in formation of such emissions is visible on the contours which agree well with the corresponding data in the literature.

**TABLE 1.** OM-355 Mercedes Benz diesel engine specifications

Engine type	Heavy duty D.I diesel engine	Injection pressure	195 bar
Number of injector holes	4	Max out put power	240 (hp)
Engine speed at max torque	1400 (rpm)	Max outlet torque	824 (N.m)
Engine speed at max power	2200 (rpm)	Number of cylinders	6,vertical type
Piston diameter × stroke	150 × 128 (mm × mm)	Compression ratio	16.1:1
Cylinder volume	11.58 (lit)		

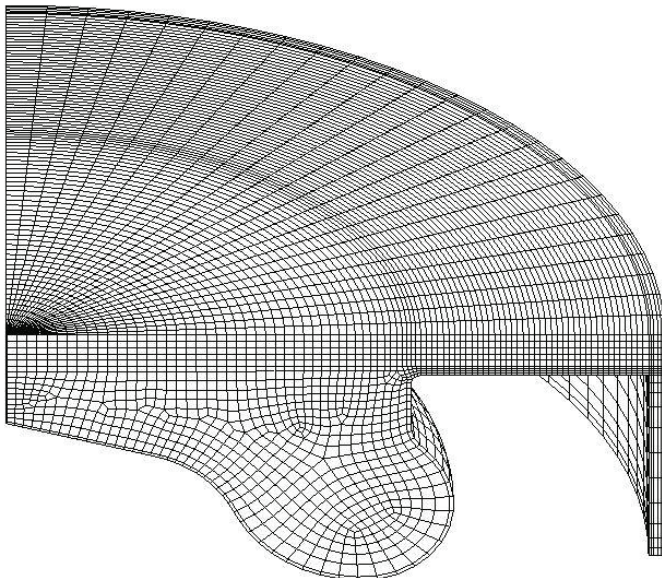


Fig. 1. Computational Mesh

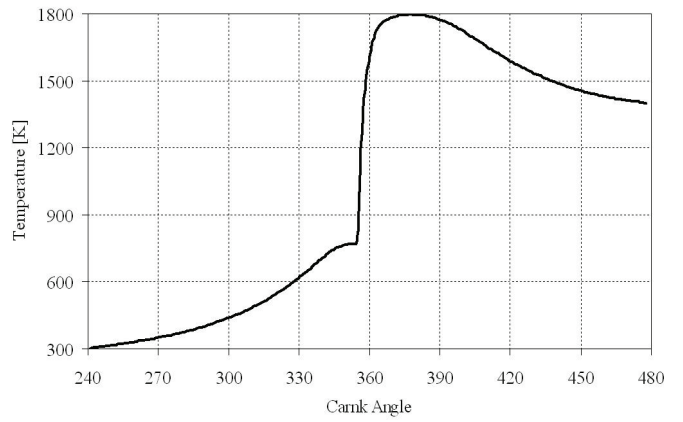


Fig. 4. Mean in-cylinder temperature change versus crank angle at 1400 rpm

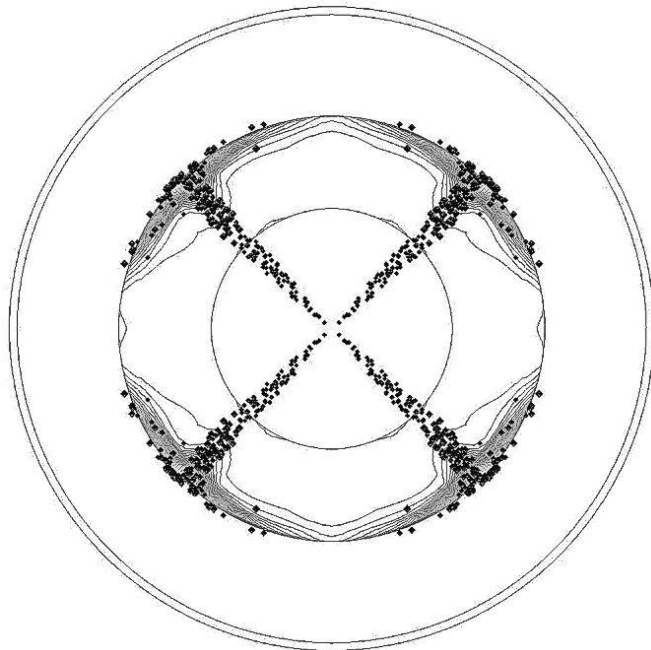


Fig. 2. Droplet distribution, fuel vapor and wall impingement at 355 °CA

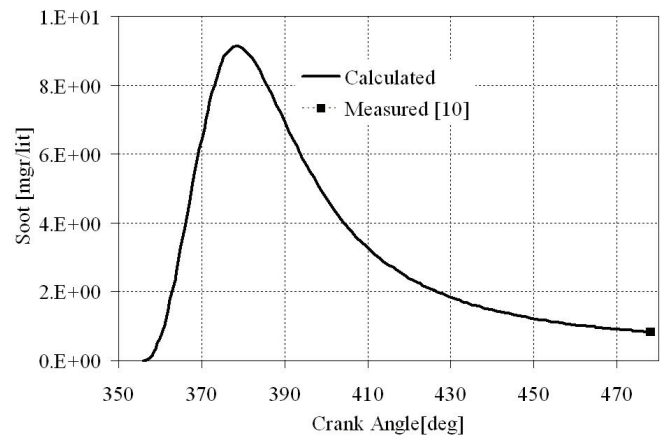


Fig. 5. Calculated and measured Soot emission comparison

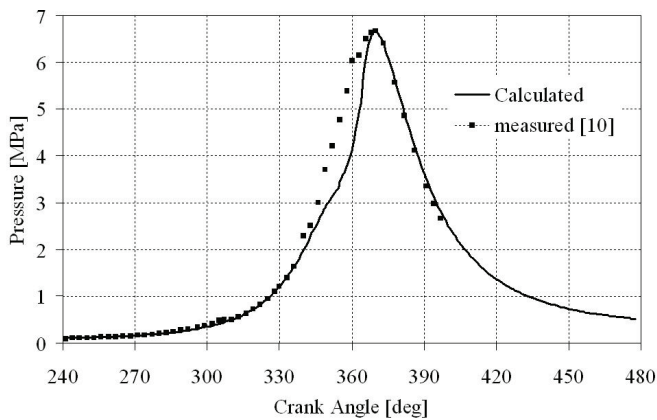


Fig. 3. CFD model and Experimental Pressure data comparison at engine speed of 1400 rpm

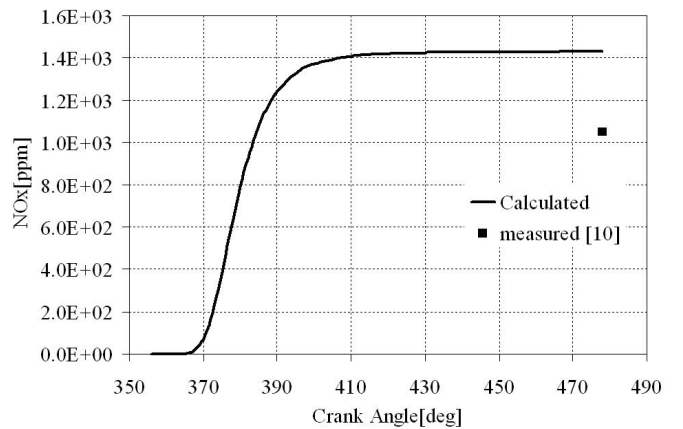
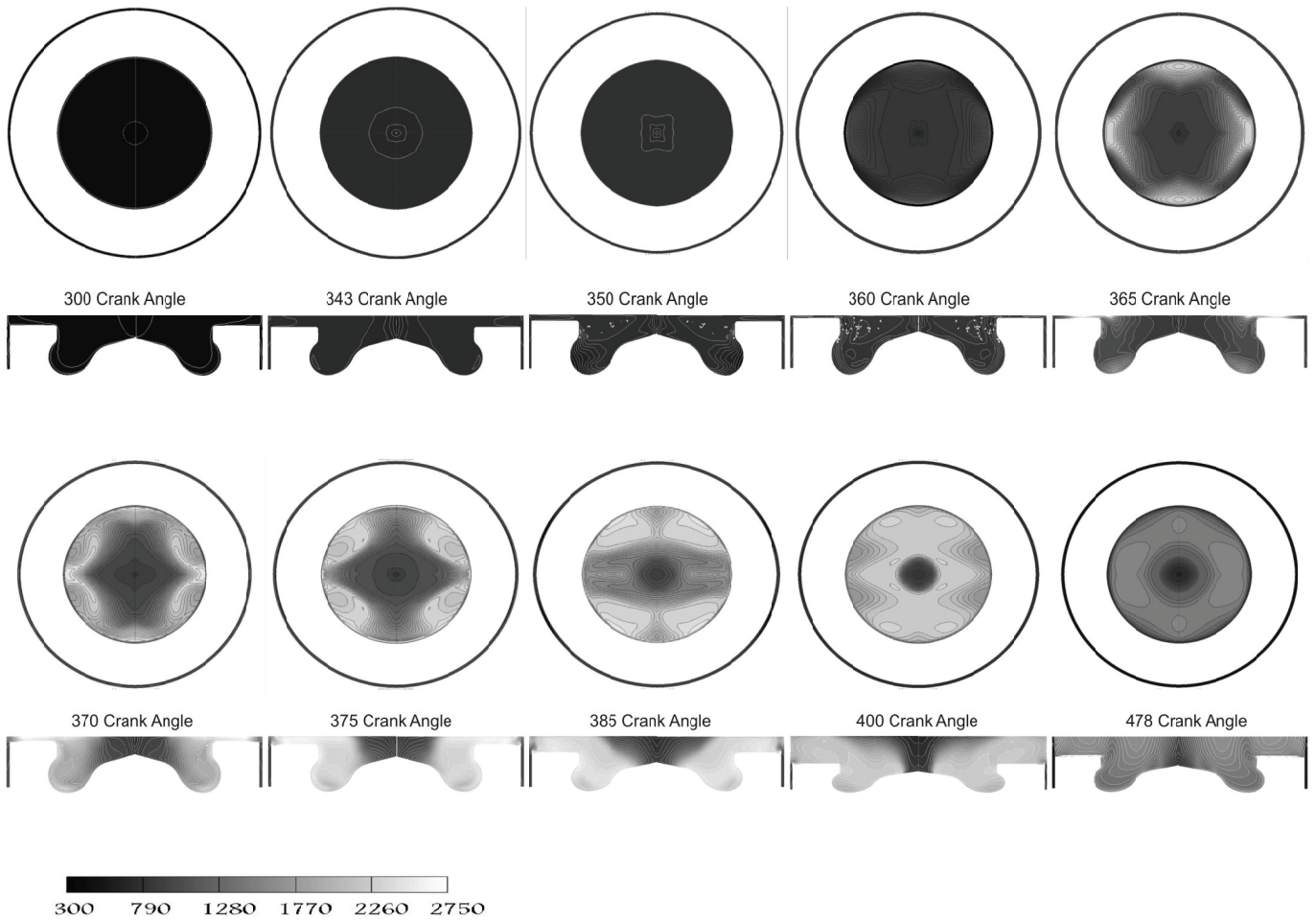
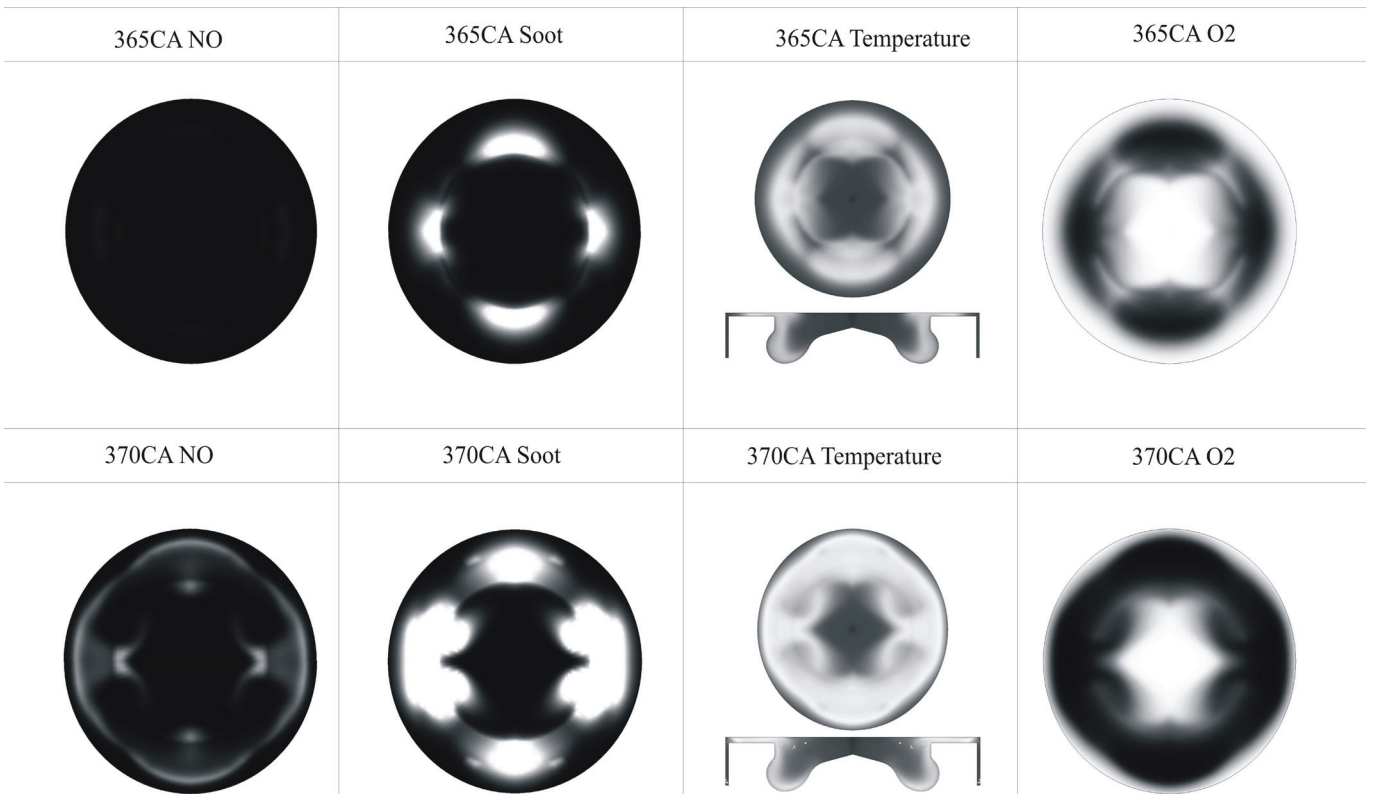


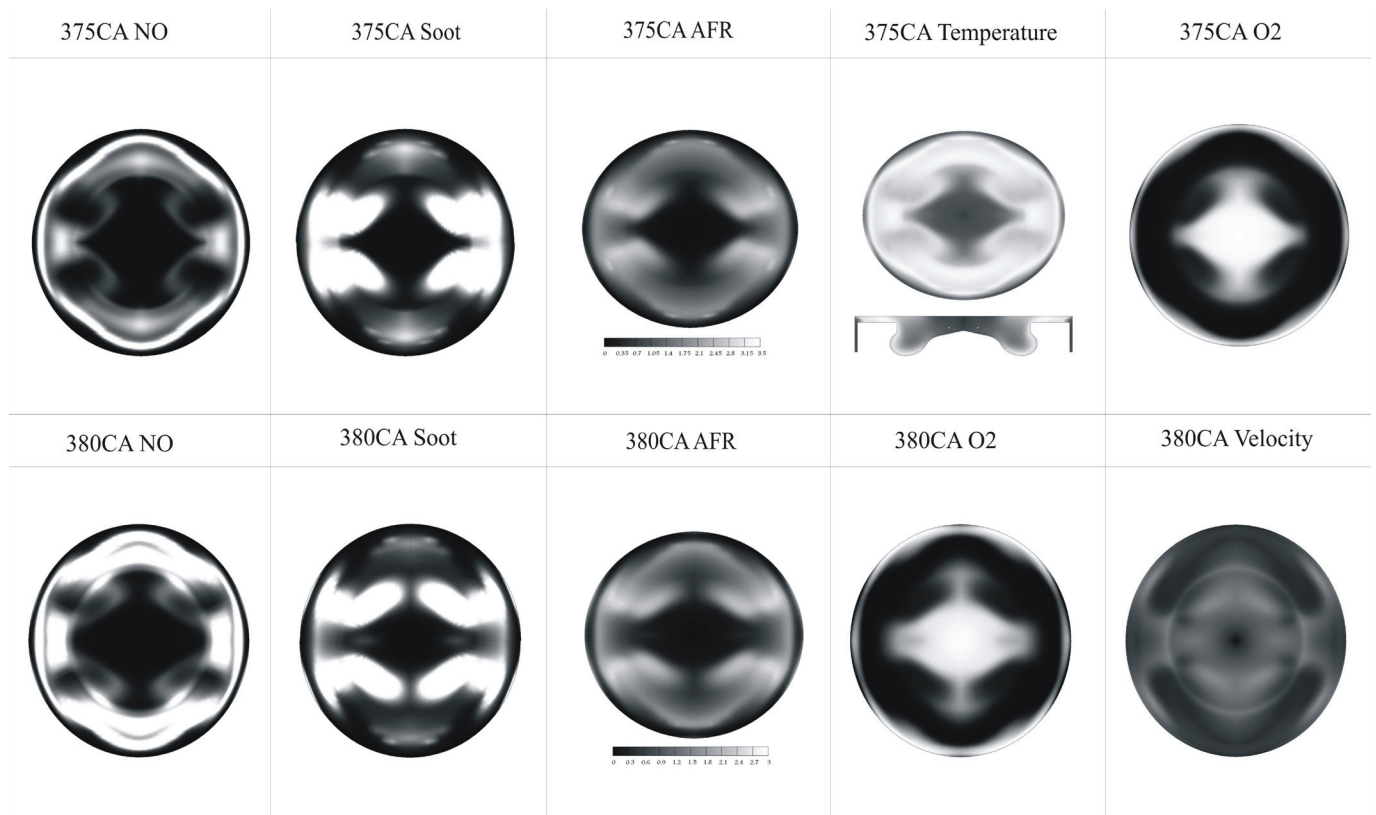
Fig. 6. Calculated and measured NO<sub>x</sub> emission comparison



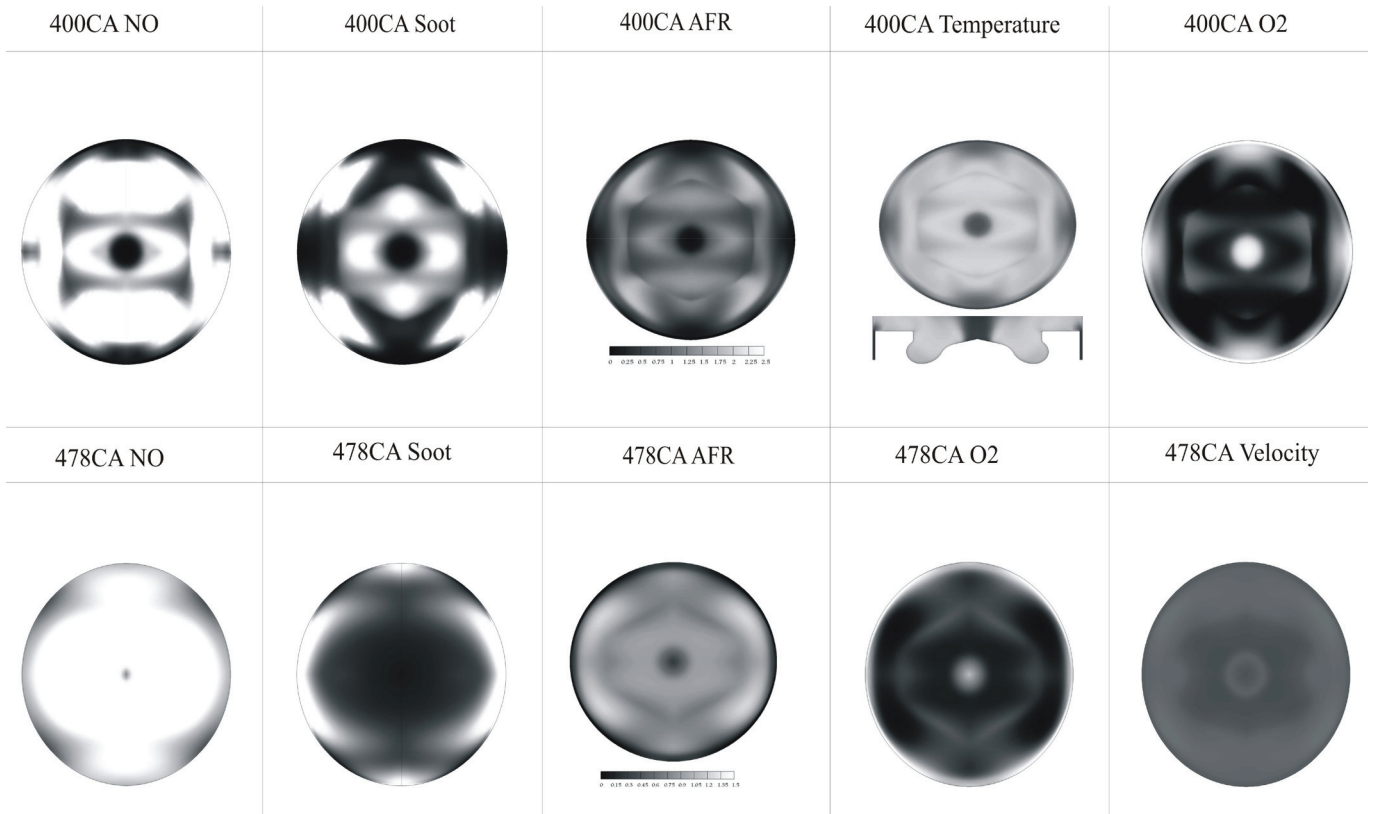
**Fig. 7.** contours of temperature in two sections for different crank angles



**Fig. 8.** Contours of Emissions, AFR, O2 and temperature at different crank angles



**Fig. 9.** Contours of Emissions, AFR and O<sub>2</sub> at different crank angles



**Fig. 10.** Contours of Emissions, AFR, O2 and temperature at different crank angles

## 8. Summery and conclusion

The present work was dedicated to modeling and study of combustion process and emission formation in a DI Diesel engine using Fire CFD code [7]. Results for calculated pressure and exhaust emissions comparison with experimental data show an acceptable accuracy. Also, at this model, impingement of spray with the piston walls was modeled and it was shown that soot mass fraction reaches the maximum amount at impinging zones while NO<sub>x</sub> concentration increases at high temperature locals where oxygen is available. Interactions of combustion and emission formation with other factors like AFR, oxygen availability and turbulence intensity were shown to be in well agreement with the data in the literature. Such verification between the experimental and computed results gives confidence in the model prediction, and suggests that the model may be used to explore new engine concepts and future works ■

### Subscripts:

$c$	:	carbon
$f$	:	forward
$fu$	:	fuel
$form$	:	formation
$fv$	:	fuel vapor
$ox$	:	oxidizer
$oxid$	:	oxidation
$pr$	:	product
$s$	:	soot
$t$	:	turbulent

### Nomenclature:

$C$	:	Empirical coefficient
$G$	:	Body-force production
$\hat{H}$ (J)	:	Enthalpy
$P$	:	Mean-strain production
$P$ (Pascal)	:	Pressure
$r$ (M)	:	Radius
$\dot{r}$ (kg/s)	:	Fuel consumption rate
$\hat{T}$ (K)	:	Temperature
$\hat{U}$ (m/s)	:	Velocity
$y$	:	Mass fraction
$\mu$ kg/ms	:	Laminar viscosity
$\tau_{ij}$	:	Stress tensor
$\mu_t$ kg/ms	:	Turbulent viscosity
$\tau_R$	:	Turbulentmixingtime scale
$\hat{\rho}$ kg/m <sup>3</sup>	:	Density
$\lambda$ W/m °K	:	Heat conductance

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