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Modeling of a Spark Ignition Engine Combustion: A Computational and Experimental Study of Combustion Process Effects on NO_x Emissions

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Abstract: In this study, the simulation results obtained by using the AVL FIRE code for a spark ignition (SI) engine are compared with experimental data. Computational fluid dynamics (CFD) is able to significantly reduce the number of experimental tests and measurements and lower the development time and costs. However, some parameters which are needed for CFD calculation must be achieved experimentally such as turbulence length scale. The CFD simulations demonstrated good agreement to the measured data. The Results show that, applying appropriate constants of each combustion model including eddy break up model (Ebu), probability density function (PDF) and coherent flamelet model (Cfm) causes the computational results to be in agreement with experimental results. Furthermore the results show that the nearest prediction in comparison with experimental results is by applying the Ebu model.

Key words: Spark ignition engine, computational fluid dynamics, combustion modeling

INTRODUCTION

With the improvement of science and technology in automotive industry, the optimization of combustion process for reduction of exhaust emissions and fuel consumption, is still a key point for engine manufacturers. Increasing the number of cars and consequently their pollution has forced the car manufacturer to develop new methods for decreasing emissions. One of the most dangerous emissions is NO_x and its reduction is an urgent need. Increasing environmental concerns and legislated emissions standards have led to the necessity of the improvements of combustion and the reductions of NO_x emissions in SI engines. Numerous experiments and computations have been performed by a large number of researchers to improve combustion and control exhaust pollutants in SI engines (Amer and Thirumala, 2002; Fontana *et al.*, 2003).

Modeling an internal combustion engine is a complex problem. This is due to numerous phenomena that each one related to the other. CFD codes able to solve this kind of problem require a lot of tools for the generation of detailed computing grids often reproducing a complex geometry, the use of several sub models and a correct definition of initial and boundary conditions. Thus, codes that allow modeling a variety of different engine configurations results are heavy to be managed, time consuming, not much friendly preprocessing and less dependent to experimentally determined model constants. In particular, the code sensitivity to experimental data could compromise the code prediction capability, especially in the modeling of the engine off-design behavior. In the past decade, computational fluid dynamics (CFD) has become a major tool for SI engine designers and researchers both as a design tool and as a means for better understanding the transient chemical and physical phenomena occurring within SI engines. For example, with the implementation of many improved models, the AVL FIRE computer code has been widely applied to simulations of the combustion and emissions in SI engines. Although model development and validation is time-consuming, once formulated it is much easier to make changes to the CFD model than it is to change a prototype (Fontana *et al.*, 2003).

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In recent years CFD has been successfully established for three dimensional simulations of fluid flow, mixture formation, pollutant formation and combustion in SI engines. The accuracy of the simulation results and hence their contribution to design analysis and optimization, however strongly depends on the predictive capacities of the models adopted for simulation of premixed flow, flame propagation, combustion and pollutant formation. In the last decade, intensive worldwide research has led to the development of a large number of models for the simulation of each of the above mentioned process and their implementation into the different in-house and non-commercial CFD codes. The increasing demands to provide fast and reliable answers to everyday engineering problems related to combustion system characteristics and performance, however in many cases cannot any longer be met by adopting in-house and non-commercial CFD solutions. Workflow integration, application specific user interfaces, sophisticated pre- and post processing capabilities are nowadays considered of being mandatory for the applicability of CFD within the engine development process (Tatschl and Riediger, 1998).

In the context of transient IC engine simulations, FIRE has already been recognized of being the leading CFD solution in terms of above mentioned capabilities. With its open software architecture and well defined model interfaces, FIRE serves as a generic CFD platform for easy integration of all kinds of mixture formation and combustion or pollutant formation models. Additionally the CFD code FIRE also provides its own broad range of combustion and pollutant formation models.

MATERIALS AND METHODS

Experimental Data

Experimental data were used both to set the initial conditions of calculation and to verify the calculated data. Measurements were made in IKco 4-cylinder production engine (ROA OHV). Engine specifications are shown in Table 1. The engine used in this study was MPFI gasoline engine. It should be noted that the experimental data were achieved from Irankhodro Engine Research, Design and Production Company (IPCO).

Computational Method Description

After performing the modeling process of combustion chamber, the meshing procedure is done by ICEM- CFD code on the combustion chamber and then the simulation and analysis of fluid and combustion behavior of the engine during the compression and expansion stroke is done by using the AVL-FIRE code.

The combustion chamber is non-symmetric, thus it is necessary to carry out a simulation over the entire domain. The chamber is divided into three characteristic volumes:

Table 1: Engine specifications

Type	4 in-line-cylinder
Bore	87.34 mm
Stroke	70.8 mm
Compression ratio	10.37
Connecting rod length	137.95 mm
Piston pin offset	0.8 mm
Intake valve opening	12.0aTDC
Intake valve closing	32.0aBDC
Exhaust valve opening	29.0bBDC
Exhaust valve closing	14.0bTDC
Maximum valve lift	6.15 mm
Ignition timing	24.0bTDC

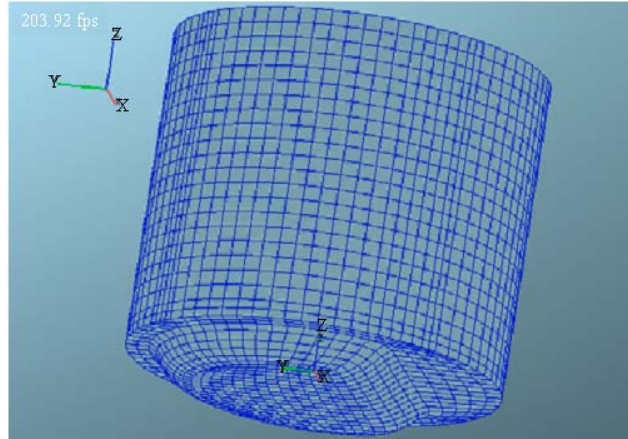


Fig. 1: The meshing of the combustion chamber when the piston is located at the position of BDC

- The bowl volume that is the cavity in the piston crown
- The clearance volume that is the volume between piston edge and cylinder head when piston located at TDC
- The squish volume that is the volume over the piston and is varying during the simulations

Every run is done with a fixed time step equivalent to 0.5 crank angle degrees. Ignition is modeled by defining the spark location and the spark advance. In AVL FIRE code an initial flame kernel, whose size value is set to 0.003 m is used.

As shown in Fig. 1, the meshing of the combustion chamber when the piston is located at the position of bottom dead center (BDC) is shown. It should be noted that the position of piston at BDC, is considered to be 180 degrees of crank angle. The computational step is started when the inlet valve closed (IVC) equal to 212 CA. At this time all the scalar variables are considered to be uniform and a number of initial points are provided by the experimental data and continues to the position that the exit valve opened (EVO) equal to 511 CA. The process of creating the moving mesh for compression stroke is performed in three steps:

- Creating the moving mesh from the position of 180 up to 320 degrees of crank angle considering 20 degrees for angle increment
- Creating the moving mesh from the position of 320 up to 340 degrees of crank angle considering 10 degrees for angle increment
- Creating the moving mesh from the position of 340 up to 360 degrees of crank angle considering 20 degrees for angle increment

The same procedure is done for the expansion stroke from TDC (360 CA degree) to BDC (540 CA degree).

After modeling of the combustion chamber, the initial and boundary conditions should be defined. After creating the moving mesh, the condition of the engine at the end of the induction stroke is considered as the initial condition. The initial operating conditions of the engine are shown in Table 2 and boundary conditions are shown in Fig. 2.

There are two parameters in the engines namely turbulence kinetic energy and turbulence length scale that are needed to be defined for computer code. The turbulence kinetic equation is as follows:

$$\text{TKE} = \frac{3}{2} \times u'^2 \quad (1)$$

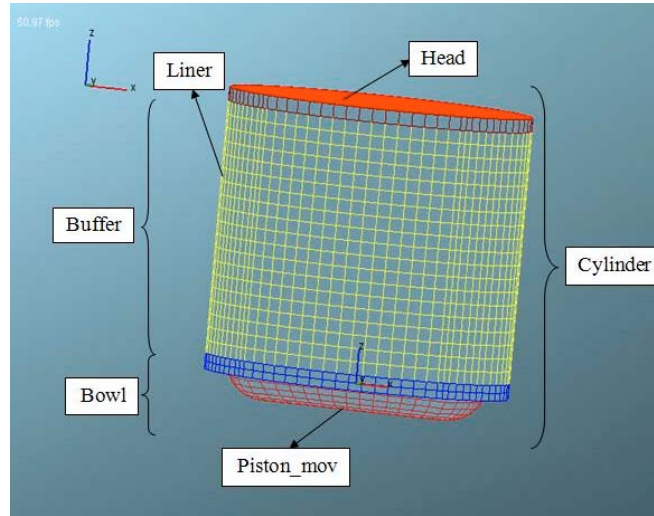


Fig. 2: Boundary conditions definition of the volume control when the piston is located at BDC

Table 2: Initial operating conditions of the engine

Variables	Values
Start angle	212 CA
End angle	511 CA
Cylinder head temperature	550 K
Cylinder liner temperature	400 K
Piston surface temperature	590 K
Cylinder pressure	97272 Pa
Inlet gas temperature	320.0 K
Engine speed	3000 rpm
Swirl ratio	1.1
Fuel type	Gasoline
Equivalence ratio	1.1
Turbulence kinetic energy	4.956 m ² sec ⁻²
Turbulence length scale	0.003075 m

where, u' is defined as follows:

$$u' = 0.7 \times (\text{mean piston velocity}) \quad (2)$$

where, mean piston velocity is defined as follows:

$$\text{Mean piston velocity} = \frac{2 \times n \times S}{60} \quad (3)$$

where, n is the engine speed equals to 3000 rpm and S is the stroke of the engine that equals to 0.0708 m.

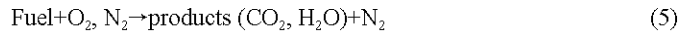
And turbulence length scale is defined as:

$$TLS = \frac{h_v}{2} \quad (4)$$

where, h_v is maximum valve lift that for OHV engine is equal to 0.00615.

Combustion Models Description

The simulations are performed by the standard release 8.31 of the AVL FIRE code. The FIRE combustion module provides a comprehensive set of models of different levels of complexity for fast and easy analysis and optimization of spark ignition engine flame propagation including assessment of knocking combustion tendency. Eddy breakup, coherent flame and transported multi-scalar PDF models are a sound basis for simulating homogeneous or non-homogeneous and stratified charge SI engine conditions. The processor allows solving the ensemble averaged governing equations of the flow and the heat transfer within the computational domain. The complex oxidation process of gasoline fuel during the turbulent combustion process is modeled by a single step irreversible reaction (Eq. 5), then five chemical species (Fuel, O₂, N₂, CO₂ and H₂O) are considered.



Three transport equations for the density weighted mean quantity fuel mass fraction, mixture fraction and residual gas mass fraction are solved together with five algebraic expressions to determine the other mass fraction as in Spalding. The solution of this set of equations depends on the determination of the mean reaction rate of Eq. 5 (Barths *et al.*, 1998; Kong *et al.*, 2001).

Three different models used to evaluate the mean reaction rate are: probability density function approach (PDF) (Fontana *et al.*, 2003; Kalio and Turunen, 1998; Tatschi and Riediger, 1998) the coherent flamelet model (Cfm) (Choi and Huh, 1998) and the turbulence controlled combustion model (Ebu) (Magnussen and Hjertager, 1977). As described by Magnussen and Hjertager (1977), the EBU model that assumes the reactants and the hot combustion products are contained in separated eddies. The chemical reactions usually have time scales that are very short in comparison to the characteristics of the turbulent transport processes. Thus, it can be assumed that the rate of combustion is determined by the rate of intermixing on a molecular scale of eddies containing reactants and those containing hot products. The useful feature of this model is that it does not call for predictions of fluctuations of reacting species. The mean reaction rate can thus be written in accordance with Magnussen and Hjertager (1977) (Eq. 6):

$$\overline{\rho_{\text{fu}}} = \frac{C_{\text{fu}}}{\tau_{\text{R}}} \overline{\rho} \min \left(\overline{y_{\text{fu}}}, \frac{\overline{y_{\text{O}_2}}}{S}, \frac{C_{\text{Pr}} \overline{y_{\text{Pr}}}}{1+S} \right) \quad (6)$$

where, $\overline{y_{\text{fu}}}$ and

$$\frac{\overline{y_{\text{O}_2}}}{S}$$

simply determine whether fuel or oxygen is present in limiting quantity and

$$\frac{C_{\text{Pr}} \overline{y_{\text{Pr}}}}{1+S}$$

is a reaction probability which ensures that the flame is not spread in the absence of hot products. C_{fu} and C_{Pr} are empirical coefficients and τ_{R} is the turbulent mixing time scale for reaction. The value of the empirical coefficient C_{fu} depends on turbulence and fuel parameters. Hence, C_{fu} requires adjustment with respect to the experimental combustion data for the case under investigation (for engines, the global rate of fuel mass fraction burnt).

The PDF combustion model takes into account the simultaneous effects of both finite rate chemistry and turbulence, thus obviates the need for any prior assumptions as to whether one of the

two processes is limiting the mean rate of reaction. Additionally, benefits of the PDF approach lie in the fact that it provides a complete statistical description of the scalar quantities under consideration. In this method, the thermo chemistry of the reactive mixture is expressed in terms of a reaction progress variable c (which is algebraically related to y_{Pr}), the mixture fraction f and the enthalpy in order to account for non-adiabaticity and bulk compression effects on temperature. The reaction progress variable c is defined as (Eq. 7):

$$c = \frac{y_{Pr}}{y_{Pr,\infty}} \quad (7)$$

where, $y_{Pr,\infty}$ is the maximum product mass fraction to occur, so that either all the fuel or all the oxidant is depleted (or both for stoichiometric mixtures). The variable c is bounded by the values of zero and unity, corresponding to fully unburned and burnt states regardless of equivalence ratio. The current method solves a transport equation for the joint probability density function $p(\varphi)$ of the mixture fraction f , the reaction progress variable c and the enthalpy h by means of a Monte Carlo Simulation technique. This enables accurate determination of the chemical sources in terms of the instantaneous thermochemical quantities of the reactive system. The term that expresses the effect of chemical reaction is modeled so that the temporal derivative of c depends on the reaction rate of Eq. 5 predicted by the chemical kinetic law (Arrhenius form, Eq. 8):

$$\omega_p = A [C_n H_m]^x [O_2]^y \cdot \exp\left(-\frac{E_a}{RT}\right) \quad (8)$$

The term representing the turbulent mixing between reactants, products and intermediate states is modeled by means of a stochastic mixing model. The modeling depends on the mixing time τ_R and the empirical constant C_{pdf} .

A turbulent premixed combustion regime can be specified using different properties such as chemical time scale, integral length scale and turbulence intensity. With the assumption that, in many combustion devices the chemical time scales (e.g., reciprocating internal engines) are much smaller in comparison to the turbulent ones, an additional combustion concept can be applied: the coherent flame model or CFM. The CFM is applicable to both premixed and non-premixed conditions on the basis of a laminar flamelet concept. The velocity S_L and thickness δ_L are mean values that integrated along the flame front which only dependent on the pressure, the temperature and the richness in fresh gases. This is a useful model since a decoupled treatment of chemistry and turbulence is considered. All flamelet models assume that reaction takes place within relatively thin layers that separate the fresh unburned gas from the fully burnt gas. Using this assumption the mean turbulent reaction rate is computed as the product of the flame surface density Σ and the laminar burning velocity S_L (Eq. 9):

$$\overline{\rho_{f_{fr}}} = -\omega_L \Sigma \quad (9)$$

where, ω_L is the mean laminar fuel consumption rate per unit surface along the flame front. For lean combustion (Eq. 10):

$$\omega_L = \rho_{f_{fr}} S_L \quad (10)$$

where, $\rho_{f_{fr}}$ is the partial fuel density of the fresh gas that is defines as (Eq. 11):

$$\rho_{f_{fr}} = \rho_{fr} Y_{f_{fr}} \quad (11)$$

where, ρ_{fr} is the density of the fresh gas and y_{fr} is the fuel mass fraction in the fresh gas. When combustion starts new terms are computed: source terms and two quantities in order to use Eq. 6: Σ and S_L .

Pollutant Model Description

Complex chemical schemes are strongly dependent on the local temperature, pressure and gas composition. Knowledge of these properties allows an accurate determination of the pollutants. In spite of this, for saving computing time mostly schemes with limited steps and species are considered for simulation.

Two different kind of chemical mechanisms are considered where the reactions in the burnt gas are assumed to be a bulk reaction which means that no local reaction zone is taken into account. These reactions are computed using the properties of the burnt gas phase, so that reactions in high temperature region are effectively computed while in the unburned regions the reaction rates are totally negligible.

For the first chemical scheme it is assumed that the reactions are very fast and the participating species are in equilibrium. The following reactions are considered using the Meintjes/Morgan mechanism for computation at the burnt gas temperature (Eq. 12):



This equilibrium mechanism solves molar concentrations of the participating species. Additionally, four equations are required in order to solve these ten concentrations and these equations are the element conservation relations for C, H, O and N. First the equilibrium constants K_C are calculated by the Eq. 13:

$$K_C^r = \exp(A_r \ln T_A + B_r/T_A + C_r + D_r T_A + E_r T_A^2) \tag{13}$$

where, $T_A = T/100$ K and A_r to E_r are constants for each reaction r .

Then the element conservation equations involving nitrogen which is uncoupled from the remainder of the system are solved for the molecular and atomic nitrogen. The eight remaining equations are then algebraically combined in order to obtain two cubic equations with two unknowns which represent the scaled concentrations of atomic hydrogen and carbon monoxide. The simultaneous cubic equations are solved using a Newton-Raphson iteration loop with scaled concentrations from the previous time step as initial values. The second mechanism calculates the NO formation using the classical extended Zeldovich scheme as follows (Eq. 14):





where, the reaction rates $\omega_{NO,r}$ for each reaction r considering both formation and destruction of NO, respectively.

The reaction rate ω_i of each participating species i in the reaction r using the stoichiometric coefficients $\nu_{i,r}$ can be written as (Eq. 15):

$$\omega_i = \sum_{r=1}^3 \nu_{i,r} \omega_{NO,r} \quad (15)$$

These two mechanisms are solved in a sequential way for computational effectiveness. It is assumed that species with low concentrations are in stationary state and their mass fractions remain at their equilibrium values during the kinetic phase. On the other hand, Complex kinetic mechanisms are applicable only for simple flame computations e.g., one dimensional, laminar and etc. For real turbulent flame calculations, their use is impractical due to the complexity of the interacting processes which must be considered to obtain realistic results. Therefore, simplified approaches must be used for complex applications, whereby essential information is not lost due to the reduction procedure.

A model derived by systematic reduction of multi-step chemistry is used in AVL FIRE code for the evaluation of the nitric oxide formation. This reduction is based on the partial equilibrium assumption of the considered elementary reactions using the extended Zeldovich mechanism describing the thermal nitrous oxide formation.

In the FIRE combustion models, an irreversible single step reaction mechanism is used for the conversion of fuel, involving only stable molecules such as C_nH_m as fuel, O_2 , CO_2 , H_2O and N_2 . Hence, an approach is implemented based on these stable molecules in order to predict thermal NO.

RESULTS AND DISCUSSION

As described previously, the result of every combustion model depends on an empirical constant (C_{Ebu} , C_{cfm} , C_{pdf} and τ). As usual, this parameter was tuned in a single engine operating point. The constants values that were obtained for each combustion models are shown in Table 3. Since, the modeling of the flame propagation depends on the characteristic mixing time scale used, two possibilities are considered. The first one assumes that the mixing time is determined by the local value of the ratio of the turbulent kinetic energy to its dissipation rate (local assumption). The second one assumes that τ_m is determined by a mean value of k-ε calculated in the computational domain (global assumption).

As it is shown in Fig. 3-5, the cylinder pressure obtained versus crank angle are shown. The results are obtained to reach maximum brake torque at the 3000 rpm of the engine speed. The results are compared to the mean pressure curves acquired in each cylinder. According to experimental results maximum cylinder pressure takes place in cylinder number 3 that is equal to 61.146 bars at 372.8 CA degrees.

Table 3: Constant values used for the combustion models

FIRE Ebu	C_{ebu} with local τ_m	14.00
	C_{ebu} with global τ_m	19.00
FIRE Cfm	C_{cfm} with local τ_m	1.44
	C_{cfm} with global τ_m	1.56
FIRE PDF	C_{pdf} with local τ_m	5.70
	C_{pdf} with global τ_m	8.00

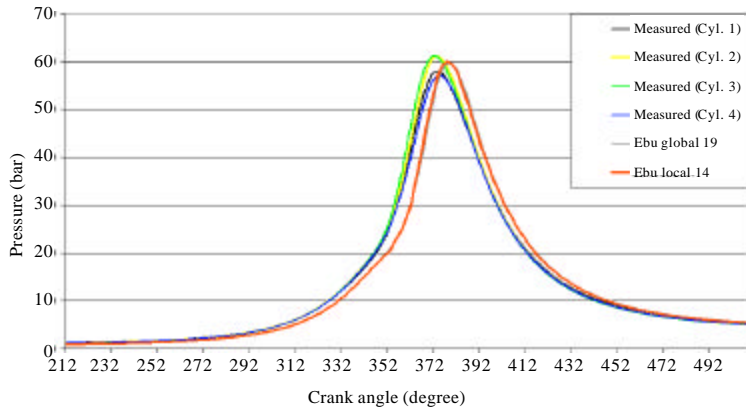


Fig. 3: Comparison between pressures curves calculated with local and global assumption for Ebu combustion model

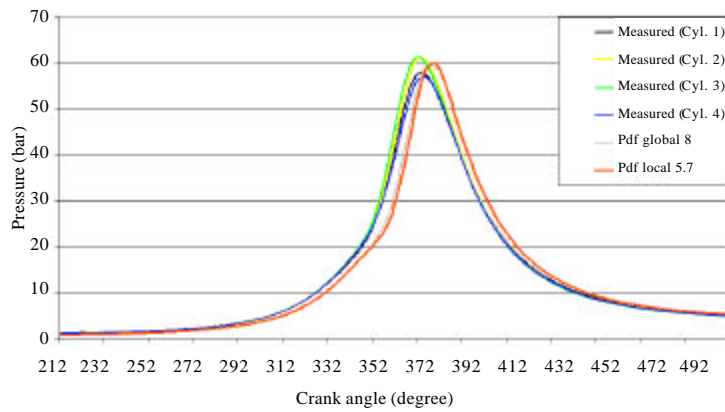


Fig. 4: Comparison between pressures curves calculated with local and global assumption for Pdf combustion model

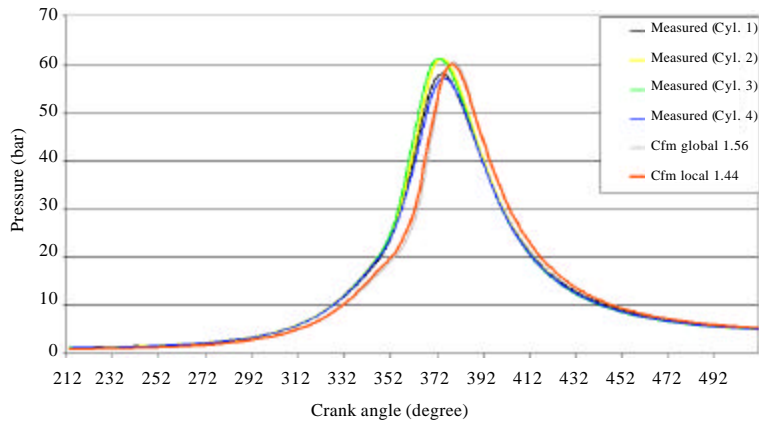


Fig. 5: Comparison between pressures curves calculated with local and global assumption for Cfm combustion model

As it can be seen from Fig. 3, the maximum cylinder pressure obtained from numerical analysis in Ebu combustion model is 59.966 bars that take place at 379 CA degrees. It should be noted that the difference between the results of global and local assumption in this combustion model is negligible. On the other hand, using the constant value of 19 for global assumption can nearly lead to the same results for constant value of 14 in local one.

Figure 4 shows that the maximum cylinder pressure obtained from numerical analysis in Pdf combustion model is 59.777 bars that take place at 381 CA degrees.

As shown in Fig. 3, the maximum cylinder pressure obtained from numerical analysis in Cfm combustion model is 59.705 bars that take place at 380 CA degrees.

The experimental value of pressure of the four cylinders at 3000 rpm is reported in Table 4. The peak pressure took place in about 373°C A because there is a short delay in ignition of air/fuel mixture to increase the pressure. The differences which takes place in cylinder peak pressure and its CA degree is because of differences in air/fuel ratio and the amount of mass entered to cylinder and the differences in convection heat transfer in each cylinder.

The variation of the calculated peak pressure with respect to the characteristic constant is reported in Table 5 for each model.

According to Table 5, the constant value is changed from -15 to 15% in comparison to the baseline case. According to the results of pressure values for these three combustion models it can be seen that the Ebu combustion model has the least difference to the experimental results.

The values of NO_x emissions for three combustion models and two assumption of local and global are shown in Fig. 6. As it can be seen the amount of NO_x in the beginning of the cycle up

Table 4: Experimental result for ROA-OHV at 3000 rpm

Cyl.	Peak pressure (bar)	Crank angle (degree)
1	57.891	374.4
2	61.084	374.0
3	61.146	372.8
4	57.006	375.2

Table 5: The model sensitivity evaluated for different values of the model constant

	Sensitivity combustion models	Peak pressure (bar %)	Peak angle (degree %)
FIRE Ebu	Local	1.14	1.23
	Global	0.39	1.29
FIRE Cfm	Local	1.81	1.46
	Global	1.79	1.28
FIRE PDF	Local	1.06	1.55
	Global	0.74	1.03

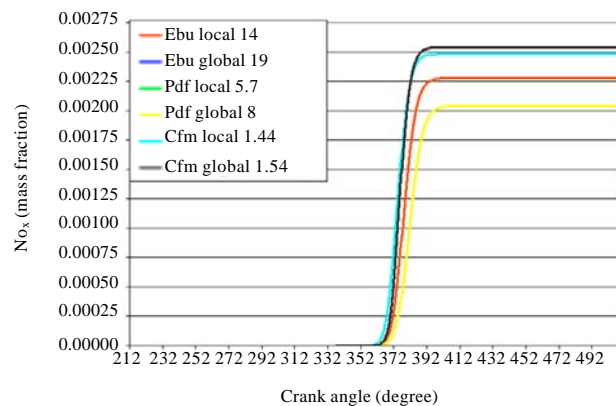


Fig. 6: Results from numerical modeling for NO_x pollution

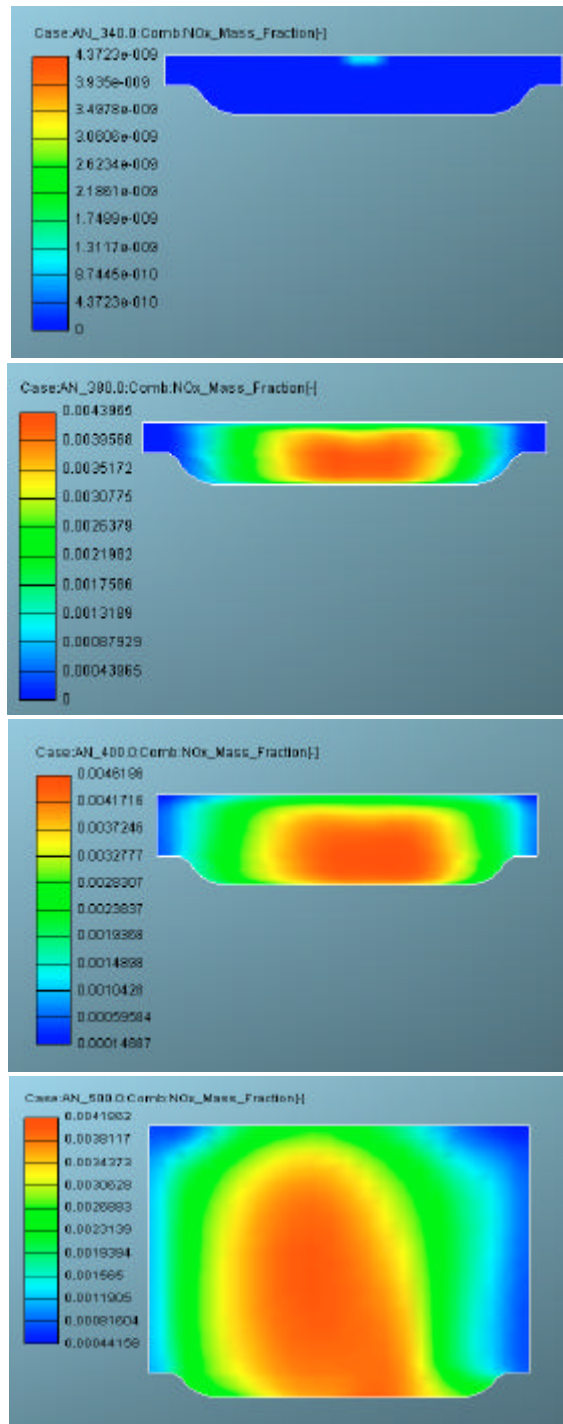


Fig. 7: The contour plot of NO_x for eddy brake up combustion model with local assumption

to 365 degrees of CA is zero and after that increases rapidly. This is because of the dependence of NO_x pollution to temperature which is raised due to start of combustion. Also after 390 degrees of CA it is constant because the temperature is due to end of combustion constant.

According to the results, the Eddy break up model with local assumption has the least variation in comparison to the experimental results. Also the results of Eddy break up model for global assumption and results of Cfm model for local assumption is coincide with each other. This behavior is observed for the results of local assumption of Pdf model and global assumption of Cfm model.

The amount of NO_x emission achieved from the experimental results is 101.08 g h⁻¹ cycle⁻¹ and for the Ebu combustion model with local assumption is 101.68 g h⁻¹ cycle⁻¹ that is the best models to describe the combustion process for NO_x emission. Figure 7 shows the contour plot for NO_x emissions of this combustion model.

CONCLUSION

With respect to results of numerical simulation, it can be concluded that numerical methods have a high capability to predict the combustion process in internal combustion engines. So that this method can be used as an appropriate means together with the experimental methods that merely is applicable by spending a lot of time and expenses. This study has shown that AVL FIRE computer code referring to the test case, are able to reproduce engine pressure cycles at different speeds and full load conditions. The results obtained are satisfying and lie within the computed and measured premixed charge range of engine cycle variation.

According to the results of pressure values for three combustion models the Ebu combustion model has the least difference to the experimental results and the Eddy break up model with local assumption has the least variation in comparison to the experimental results.

Results from numerical modeling for NO_x pollution is 101.68 g h⁻¹ cycle⁻¹. Error in calculating NO_x pollution in comparison to the experimental results is 0.6% which indicates a good consistence.

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