World Applied Sciences Journal 18 (7): 890-895, 2012
ISSN 1818-4952

DOI: 10.5829/idosi.wasj.2012.18.07.1985

Three Dimensional Modeling of Combustion Process and Emission Formation in a Spark Ignition Engine

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Abstract: This paper is presented to numerically study the combustion process and pollutant formation in the Samand XU7 JP Spark Ignition (SI) engine at various engine speeds. The computations are carried out using a three-dimensional model for flows, combustion and emissions in SI engines. Four engine speeds have been studied: 1500, 2000, 3000 and 4000 rev/min. The obtained results indicate that spark timing should be advanced by increasing engine speed and ignition delay and combustion duration are increased respectively. Also by increasing engine speed from 1500 rev/min to 4000 rev/min CO quantity increases about 40 percent and NOx quantity increases about 2.5 times. The obtained results are compared to the experimental data measured at Iran Khodro Powertrain Company (IP-CO) for in-cylinder pressure and emissions at various engine speeds. There is a good agreement among the results. The simulation results show that the CFD combustion simulation tool, works quite correctly for the predicting combustion process and emission formation in Samand SI engine.

Key words: SI engine · Spark Ignition · Combustion · CFD · Pollutant

INTRODUCTION

Internal combustion engines have proved very practical and useful due to the high efficiency and considerable power to weight ratio and volume and are widely used in many fields such as transportation, automotive industry, etc. Nowadays, because of the crisis of depletion of energy resources and environmental dilemmas, a lot of researches are being done to improve thermal efficiency and to control and reduce emission trade-off on such engines. There has been a lot of works done in the field of engine research using both thermodynamic methods and computer aided modeling and simulations. With the progressive development of computational fluid dynamics (CFD) and flow field models, it is possible to study and predict droplet distribution, temperature, pressure and other parameters at every desired point and time within the combustion chamber.

In experimental investigations measuring of the flame propagation in combustion chamber in SI engines is too difficult, but Three-dimensional modeling easily allows studying on the flame propagation and its significant effect on combustion parameters and emission formation process.

A lot of researches have been done on in-cylinder flow field and its effects on overall engine processes. Combustion rate, air-fuel mixture, pollution formation and efficiency in a Spark Ignition (SI) engine is quite depend on in-cylinder flow field. Flow field models, such as KIVA II code in 1990 [1, 2] and numerical Ricardo Code in 1992 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 [3], are premiere examples.

In 2001, Fontana *et al*. [4] have simulated a four cylinder spark ignition engine using AVL Fire CFD code. Comparing the obtained numerical results to experimental data indicated the ability of AVL Fire code in predicting the engine processes. At this investigation, three combustion models (Eddy-Breakup, PDF and CFM) are utilized to simulate the combustion process. Also the obtained results from AVL Fire are compared to KIVA-3V code and are showed a good agreement in pressure and NO_x pollutant.

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Zhichao Tan and R.D. Reitz [5] have studied an ignition and combustion model based on the level-set method for spark ignition engine multidimensional modeling using KIVA-3V CFD code. C-M. Wu *et al*. [5] have investigated effects of engine speed on combustion in SI engines using quasidimensional fractal engine simulation (UT-FES). Comparisons of the predictions of the UT-FES code with experimental data showed that this model was able to predict the effects of load and equivalence ratio, but did not predict the effects of speed as accurately.

Reinhard Tatschl and Hannes Riediger [6] have studied PDF (Probability Density Function) modeling of stratified charge SI engine combustion which is implemented into the CFD code Fire. In another work, L. Andreassi *et al*. [7] have improved the KIVA-3V code to analysis the 3D simulation of SI combustion. Comparisons between two different turbulent combustion models have been performed and have concluded that Cant model seems to exhibit more predicting reliability in the whole engine operating field.

Fredric Westine *et al*. [8] have simulated a turbocharged SI engine with two different 1D engine simulation software (GT-Power and Virtual Engines) and compared the results with measured data.

At the present work a three dimensional AVL Fire v8.3 CFD code has been used to predict and study the combustion process and emissions formation at different engine speeds in the Samand XU7 JP SI engine. This paper also demonstrates the usefulness of multidimensional models to gain insight into the combustion process and to provide direction for exploring new engine concepts. The obtained results are compared to experimental data measured at Iran Khodro Powertrain Company for in-cylinder pressure and emissions at various engine speeds. There is a good agreement among the results.

Model Formulation: The numerical model for light duty Samand XU7 JP SI engine with the specifications on table 1 is performed by using AVL Fire code. Calculations are carried out on the closed thermodynamical system from Intake Valve Closure (IVC) at -150°CA to Exhaust Valve Opening (EVO) at 140°CA. Figure 1 shows the numerical grid which is designed to model the geometry of the engine and contains a maximum 77,000 cells at BDC. The number of cells is allowed to change in compression stage. The present resolution was found to give adequately grid independent results.

Table 1: Specifications of Samand XU7 JP spark ignition engine

Number of cylinders	4
Cycle type	Four stroke
Bore [mm]	83
Stroke [mm]	81.4
Conrod [mm]	143.1
Compression ratio	9.2
Displacement Volume	1.75 Lit.
Piston pin Off [mm]	0.8
Cam Timing:	
IVO [deg] @ 1 mm lift	8.5 deg BTDC
IVC [deg] @ 1 mm lift	29.3 deg ABDC
EVO [deg] @ 1 mm lift	43.3 deg BBDC
EVC [deg] @ 1 mm lift	5.5 deg BTDC

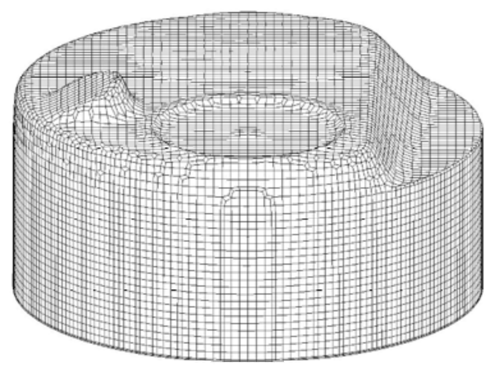

Fig. 1: Samand XU7 JP computational grid at 60 CA BTDC

The initial pressures for each case are obtained from experimental data and the initial temperatures are calculated by ideal gas law. Initial swirl ratio is set at 1.1 of engine speed for an approximately quiescent condition and Exhaust Gas Recirculation (EGR) is assumed to be zero in all cases. The studied engine speeds are 1500, 2000, 3000 and 4000 rev/min and all cases are in full load condition. All boundaries temperatures were assumed to be constant throughout the simulation, but allowed to vary with the combustion chamber surface regions.

The Equations Used by Numerical Model Are as Follows [9]:

Continuum Equation:

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

***k* – *ε* Turbulent and Momentum Equations:**

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

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

$$P=-2\mu_t S:S-\frac{2}{3}\left[\mu_t\left(trS\right)+K\right]\left(trS\right) \quad (4)$$

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

$$\mu_t=C_\mu\rho\frac{k^2}{\varepsilon} \quad (6)$$

C_μ	$C_{\varepsilon 1}$	$C_{\varepsilon 2}$	$C_{\varepsilon 3}$	$C_{\varepsilon 4}$	σ_k	σ_ε	σ_ρ
0.09	1.44	1.92	0.8	0.33	1	1.3	0.9

Energy Equation:

$$\rho\frac{DH}{Dt}=\rho\left(\frac{\partial H}{\partial t}+U_j\frac{\partial H}{\partial x_j}\right)=\rho\dot{q}_g+\frac{\partial P}{\partial t}+\frac{\partial}{\partial x_i}\left(U_j\tau_{ij}\right)+\frac{\partial}{\partial x_j}\left(\lambda\frac{\partial T}{\partial x_j}\right) \quad (7)$$

Characteristic Timescale Model (Combustion Process): The Characteristic Timescale model is utilized in this study because it is able to predict the CO emission formation while the other combustion models (such as Eddy Breakup, Coherent Flame Model and Probability Density Function) can not compute it. This model combines a laminar and a turbulent time scale to an overall reaction rate. The time rate of change of a species *m* due to this time scale can be written as follows:

$$\frac{dY_m}{dt}=-\frac{Y_m-Y_m^*}{\tau_c} \quad (8)$$

where Y_m is the mass fraction of the species *m* and Y_m^* is the local instantaneous thermodynamic equilibrium value of the mass fraction. τ_c is the characteristic time for the achievement of such equilibrium. It is sufficient to consider the seven species Fuel, O_2, N_2, CO_2, CO, H_2 and H2O to predict thermodynamic equilibrium temperature accurately enough.

Zeldovich Mechanism for NO_x Prediction: The thermal NO_x formation mechanism is expressed in terms of the extended Zeldovich mechanism [13]:

$$N_2+O\longleftrightarrow NO+N \quad (9)$$

$$N+O_2\longleftrightarrow NO+O \quad (10)$$

$$N+OH\longleftrightarrow NO+H \quad (11)$$

All above equations are taken into account simultaneously to predict combustion progress in the turbulent flow field, gasoline fuel consumption rate, flame propagation and etc., using two stage pressure correction algorithms.

RESULTS AND DISCUSSION

The calculations are carried out for the four cylinder Samand XU7 JP spark ignition engine and the operating conditions are engine speeds 1500, 2000, 3000 and 4000 rev/min at full load mode. The predictions are presented in figures below show global (cylinder averaged) quantities as a function of time (crank angle) during the closed cycle.

The model predictions are compared to the experimental pressure histories [14] in figure 2 for all the engine speeds. The accuracy of the model is evaluated by comparisons of the location of peak pressure and the magnitude of the peak pressure. There is a good agreement among the results. As can be seen when engine speed increase, because of less available time for heat transfer from the cylinder walls and higher swirl in combustion chamber which causes the fast flame propagation, pressure peak increases. Figure 2 also indicates that with the increase of engine speed motoring pressure increases.

Increasing in engine speed causes to advance ignition timing because of increasing in ignition delay. Table 2 shows the ignition timing, ignition delay and combustion duration for all studied cases. Ignition delay and combustion duration are decreased according to needed time to perform the combustion process (Table 2).

Figures 3 and 4 indicate the heat release rate and mean in-cylinder temperature histories versus crank angle. It can be seen that increasing in engine speed cause to increase in heat release rate and mean temperature. Flame propagation velocity increases with the increase of engine speed and causes the pressure, temperature and heat release rate peaks approach to TDC (Figures 2, 3 and 4).

Table 2: Ignition and combustion specifications at various engine speeds

	Ignition Timing	Ignition Delay	Combustion Duration
1500 rev/min	11 CA BTDC	7 CA= 0.777 ms	30 CA= 3.33 ms
2000 rev/min	15 CA BTDC	8 CA= 0.667 ms	30 CA= 2.50 ms
3000 rev/min	17.5 CA BTDC	11 CA=0.610 ms	32 CA= 1.78 ms
4000 rev/min	24.5 CA BTDC	13 CA=0.542 ms	36 CA= 1.50 ms

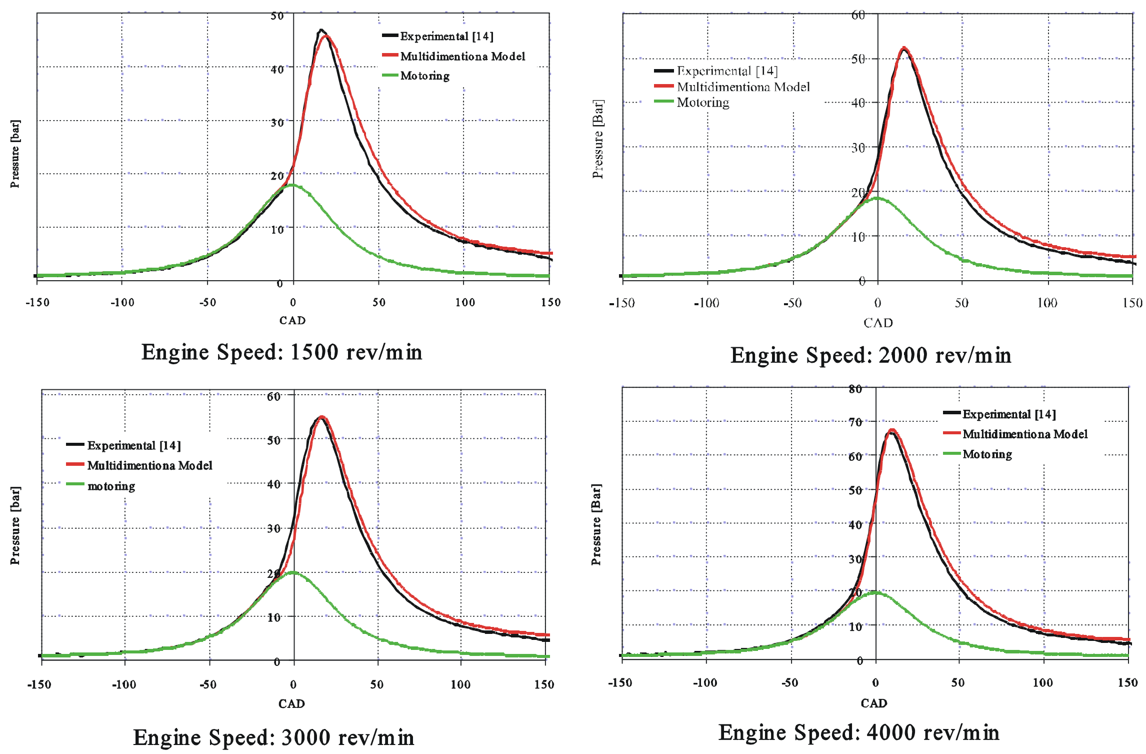

Fig. 2: Comparison of model predictions with experimental data [14] for mean in-cylinder pressure at mentioned engine speeds

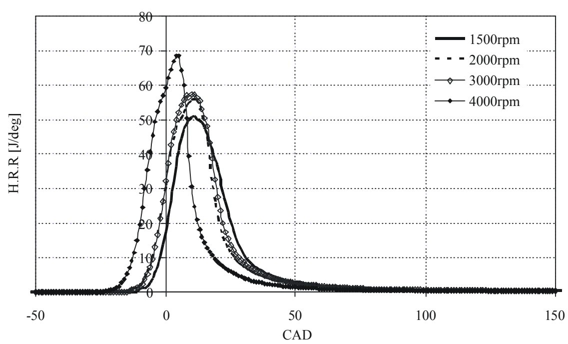

Fig. 3: Heat Release Rate versus crank angle at different engine speeds

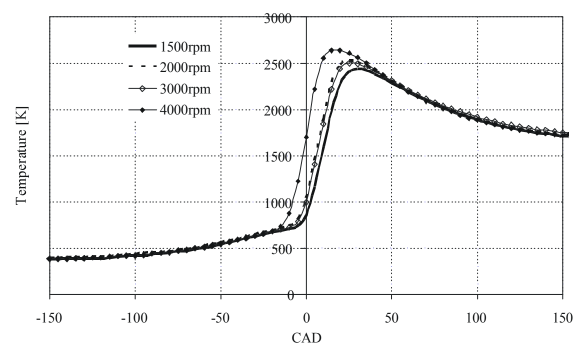

Fig. 4: Mean in-cylinder temperature versus crank angles at different engine speeds

Figure 5 represents the achieved indicated work per cycle for all cases. Negative work quantity in compression stage increases by increasing in engine speed because of less available time for heat transfer from cylinder walls and also the positive work in expansion stage increases in the same way because of higher pressure peak.

Figure 6 represents the comparison of CO concentration with the experimental data [14] at studied engine speeds. In experiment the emission concentrations are measured at the exhaust and because of that the experimental data are shown in figure 6 as points. The obtained results at 1500 and 2000 rpm have a good agreement with the experiments, but amount of error increases by increase of engine speed.

Table 3 represents the NO_x emission concentration at the exhaust valve opening (EVO) at mentioned engine speeds. The area which the equivalence ratio is close to 1 and the temperature is higher than 2000 K is the NO_x formation area [15]. It can be seen that with the engine speed increasing, this emission amount increases because of increasing in combustion chamber temperature.

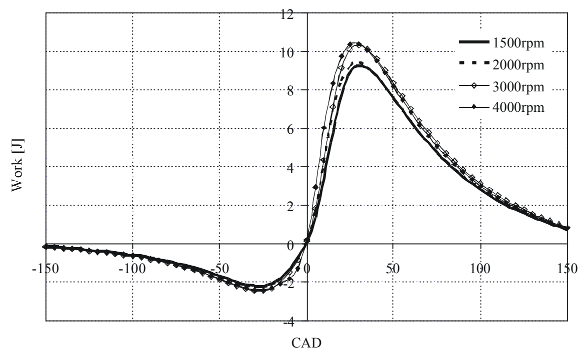

Fig. 5: Indicated work per cycle versus crank angle at different engine speeds

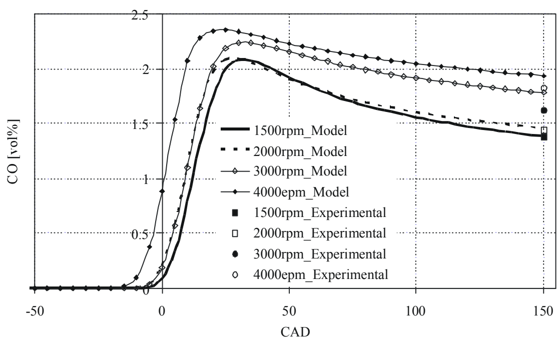

Fig. 6: Comparison of CO concentration with experimental data at mentioned engine speeds

Fig. 7: In-cylinder temperature contours at 1500 rpm

Table 3: Prediction of NO_x emission concentration at the exhaust valve opening (EVO) at mentioned engine speeds

Engine speed	NO_x emission
1500 rev/min	0.273 $^{gr}/_{kW.hr}$
2000 rev/min	0.443 $^{gr}/_{kW.hr}$
3000 rev/min	0.512 $^{gr}/_{kW.hr}$
4000 rev/min	0.723 $^{gr}/_{kW.hr}$

Figure 7 indicates the in-cylinder temperature contours at 1500rpm from the start of combustion at 5 CA BTDC until the flame takes over the whole combustion chamber. These contours can be mentioned as the flame propagation marker. For all of engine speeds these contours are the same and just differ in propagation velocity.

SUMMARY AND CONCLUSION

At the present work, effect of engine speed on combustion process and pollutant formation was numerically investigated using AVL FIRE Code. Four cases for engine speeds were studied as follows: 1500, 2000, 3000 and 4000 rev/min. The obtained results indicate that spark timing should be advanced by increasing engine speed and ignition delay and combustion duration are increased with the increase of engine speed.

Also CO quantity increases 40 percent by increasing engine speed from 1500 rev/min to 4000 rev/min and NOx quantity increases about 2.5 times. The obtained results are compared to experimental data measured at Iran Khodro Powertrain Company (IP-CO) for in-cylinder pressure and emissions and represent a good agreement.

Nomenclature:

C	Empirical Coefficient
G	Bulk Forces
$\hat{H}$	Enthalpy'J
P	Mean Strain
p	Pressure, Pa
r	Radius, m
$\dot{r}$	Fuel Consumption Rate, Kg/s
$\hat{T}$	Temperature, K
$\hat{U}$	Velocity, m/s
y	Mass Fraction

Greek Letters:

$\hat{\rho}$ Density, Kg/m3
μ Laminar Flow Viscosity, Kg/ms
μ_t Turbulent Flow Viscosity, Kg/ms
λ Heat Conductivity, J/m-K
τ_{ij} Stress Tensor
τ_R Turbulent Mixing Time Scale

Subscripts:

c Carbon
f Forward
form Formation
fu Fuel
fv Fuel Vapor
ox Oxidizer
oxid Oxidation
pr Products
s Soot
t Turbulence

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