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Study of CNG Combustion under Internal Combustion Engines Conditions.

Part II: Using of Multi-Dimensional Modeling.

In this investigation, a multi-dimensional modeling has been developed to predict the performance and pollutants emissions of an internal combustion engine (ICE). The CNG (compressed natural gas) has been used as fuel. The single step oxidation of methane with oxygen to form carbon dioxide and water vapor has been used. The produced pollutants are calculated with using the chemical kinetic and equilibrium equations (10 species, 5 elementary reactions for kinetic and 6 elementary reactions for equilibrium) and the standard k-ε turbulence model has been used in this investigation.

SYMBOLS

C_v, Cp	Specific heat capacity (Kj/Kg.K)
A_v	Area (m^2)
h	Enthalpy (Kj/Kg)
h_f	Enthalpy of formation (Kj/Kg)
F	Fuel (kg)
A	Air (Kg)
B	Cylinder bore (m)
W	Molecular weight (Kg)
m	Mass (Kg)
$\dot{m}_i$	Mass flows rate into the cylinder (Kg/s)
$\dot{m}_e$	Mass flows rate out of the cylinder(Kg/s)
V	Volume (m^3)
t	Time (s)
T	Temperature (K)
$E_{fn,rn}$	Activation energy (J/mol)
$\beta_{fn,rn}$	Reaction constant
K_{fn},K_{rn}	Reaction rate Constants

Greek Symbols

θ	Crank angle (Deg.)
φ	Equivalence ratio
ρ	Density (Kg/m^3)

Subscripts and Superscripts

g	Gas

Abbreviations

NOx	Oxides of nitrogen
TDC	Top dead center
ATDC	After top dead center
BBDC	Before bottom dead center
BTDC	Before top dead center
ABDC	After bottom dead center
ICE	Internal combustion engine
CNG	Compressed natural gas

INTRODUCTION

In engineering, modeling a process means to develop and use the appropriate combination of assumptions and equations that permit critical features of the process to be analyzed. Engine models describe the thermodynamic, fluid flow, heat transfer, combustion, and pollutant-formation phenomena in engines. Examples of labels given to engine models are zero-dimensional, quasi-dimensional and multi-dimensional models. These can also be categorized as thermodynamic or fluid dynamic in nature, depending on whether the equations which give the model its predominant structure are based on energy conservation or on a full analysis of fluid motion. In Multi-Dimensional models, the full governing differential conservation equations of physics with time and spatial dimensions are solved for the processes in the engine. Many sub-models, such as turbulence and combustion models, are still needed to avoid the need for direct calculation of the Navier-Stokes equations and chemical reactions. Detailed boundary and initial conditions are also necessary. Numerical methodologies are introduced to approximate the differential equations by their algebraic counterparts whose dependent variables are the values of the velocities, pressure, temperature, etc., at the nodal points of a computational mesh. Natural gas is an economical, clean burning fuel, whose advantages as an alternative fuel for internal combustion engines have been well documented [1-3]. Obviously knowing at what conditions of temperatures, pressures, and compositions a methane-air mixture can ignite, is very important in optimization of an engine performance. A fundamental understanding of the thermodynamics and fuel composition related factors influencing combustion in internal combustion engines can only be obtained from a detailed study of the processes. Therefore, the objective of this work is study of performance and pollutants emissions from an internal combustion engine with using multi-dimensional modeling and implementation of chemical kinetic and equilibrium equations for natural gas combustion.

Engine description

A two valve spark ignition engine has been considered and its data are shown in Table 1. Also the valves lifting variation profile is shown in Fig.1.

Cylinder bore	8.255Cm
Connecting rod	15.24Cm
Stroke	8.7075Cm
Squish	1.07Cm
Inlet valve open(IVO)	15BTDC
Inlet valve diameter	3.2Cm
Exhaust valve diameter	2.8Cm

Table 1. Engine data.

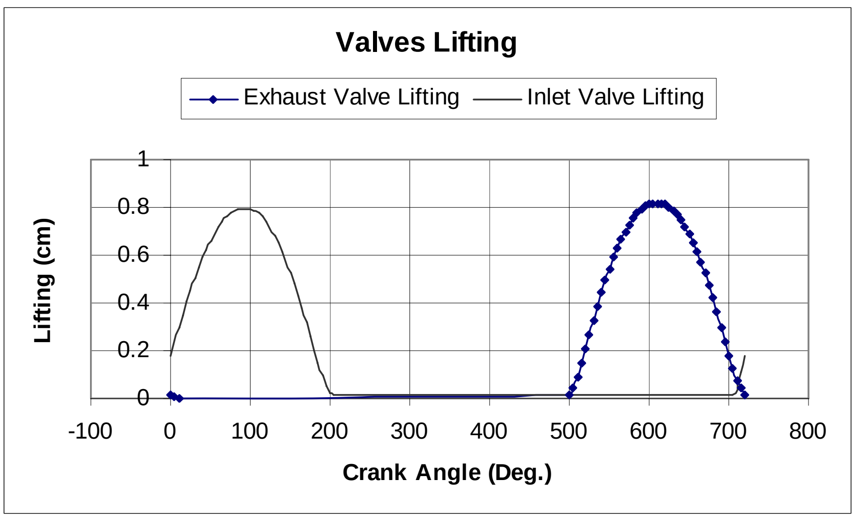

Figure 1. Valves Lifting profiles.

GOVERNING EQUATIONS

This simulation divides the complete cycle into the overlap, intake, compression, combustion, expansion and exhaust processes. In each of these processes the governing equations of fluid flow and chemical reactions are solved in a generated mesh.

Continuity Equation;

$$\frac{\partial \rho_m}{\partial t} + \nabla \bullet (\rho_m \vec{u}) = \nabla \bullet \left[\rho D \nabla (\frac{\rho_m}{\rho})\right] + \dot{\rho}_m^c + \dot{\rho}_m^s \delta_{ml} \qquad (1)$$

Momentum equations;

$$\frac{\partial}{\partial t}(\rho\vec{u}) + \nabla \bullet (\rho\vec{u}\vec{u}) = -\frac{1}{a^2}\nabla P - A_o \nabla(\frac{2}{3}\rho k) + \nabla.\sigma + \vec{F}^s + \rho g \qquad (2)$$

Turbulence kinetic equation;

$$\frac{\partial}{\partial t}(\rho k) + \nabla \bullet (\rho\vec{u}k) = -\frac{2}{3}\rho k \nabla.\vec{u} + \sigma : \nabla\vec{u} \bullet \left[(\frac{\mu}{\Pr_k})\nabla k\right] - \rho\varepsilon + \dot{W}^s \qquad (3)$$

Epsilon equation;

$$\frac{\partial}{\partial t}(\rho\varepsilon)+\nabla\bullet(\rho\vec{u}\varepsilon)=-(\frac{2}{3}C_{\varepsilon 1}-C_{\varepsilon 3}+\frac{2}{3}C_{\mu}C_{\eta}\frac{k}{\varepsilon}\nabla\bullet\vec{u})\rho\varepsilon\nabla\bullet\vec{u}$$ (4)

$$-\frac{\varepsilon}{k}\left[(C_{\varepsilon 1}-C_{\eta})\sigma:\nabla\vec{u}-C_{\varepsilon 2}\rho\varepsilon+C_{s}W^{\cdot s}\right]+\nabla\bullet\left[(\frac{\mu}{\mathrm{Pr}_{k}})\nabla\varepsilon\right]$$

Where

$$C_{\varepsilon 1}=1.42, C_{\varepsilon 2}=1.68, C_{\varepsilon 3}=0.41333+(-1)^{\delta}0.06899C_{\eta}\eta$$ (5)

$$C_{\eta}=\frac{\eta(1-\eta/\eta_{o})}{1+\beta\eta^{3}},\begin{cases}\delta=1 & \text{if}\quad \nabla\bullet\vec{u}<0\\ \delta=0 & \text{if}\quad \nabla\bullet\vec{u}>0\end{cases}$$ (6)

$$\eta=S\frac{k}{3}\quad,\quad S=(2S_{ij}S_{ij})^{1/2}\quad,\quad S_{ij}=\frac{1}{2}(\frac{\partial u_{i}}{\partial x_{j}}+\frac{\partial u_{j}}{\partial x_{i}})$$ (7)

Chemical Equations

3.1 Chemical Equilibrium

The following species has been used for compressed natural gas (CNG) combustion;

Fuel, NO, O, N2, O2, N, H2, OH, CO, CO2 and the following equations have been considered for chemical equilibrium in combustion calculations.

$$H_2 \Leftrightarrow 2H$$ (8)

$$O_2 \Leftrightarrow 2O$$ (9)

$$N_2 \Leftrightarrow 2N$$ (10)

$$O_2 + H_2 \Leftrightarrow 2OH$$ (11)

$$O_2 + 2H_2O \Leftrightarrow 4OH$$ (12)

$$O_2 + 2CO \Leftrightarrow 2CO_2$$ (13)

3.2 Chemical Kinetics

The model assumed single step oxidation of compressed natural gas (CNG) with oxygen to form carbon dioxide and water vapor;

$$CH_4 + 2O_2 \Leftrightarrow CO_2 + 2H_2O$$ (14)

The reaction rate for this single step has been used is the global one-step methane oxidation reaction rate proposed by Westbrook and Dryer [32] in standard SI units.

$$dCH_4 / dt = -130x10^{6}\exp(-24400/T)[CH_4]^{-0.3}[O_2]^{1.3}$$

Also the single step oxidation of gasoline is as blow;

$$4C_8H_{17} + 49O_2 \Leftrightarrow 32CO_2 + 34H_2O$$ (15)

The extended Zeldovich kinetic equations have been used for calculation of NO emission;

$$N_2 + O \Leftrightarrow N + NO$$ (16)

$$O_2 + N \Leftrightarrow O + NO$$ (17)

$$N + OH \Leftrightarrow H + NO$$ (18)

RESULTS AND DISCUSSIONS

In this investigation a vertical valve engine with moving boundary conditions at stems and for full circle in cylindrical coordinate has been used for mesh generation. The generated meshes and different sections are shown in Figures (2-5). The generated mesh has ability for moving grids at stems for opening and closing valves and this mesh is full dynamically.

Figures (6-9) show the velocity vectors and streamlines of fluid flow in throughout the intake process. Angular momentum variation and tumble generation in Y direction(vertical to screen) with crank angle are shown in figures 10. and 11.; in the intake stroke the angular momentum increases, because the fluid flow (air+fuel) enter into the cylinder with high speed and at special angle to valve seat. This phenomena is useful in direct injection engines for obtaining good mixing of fuel and air mixtures, because the mixing process affect the engine combustion performance very much. The angular momentum and tumble generation in Y direction decrease in compression stroke, because the top of piston has been considered flat in this modeling. The angular momentum and tumble generation stay constant throughout the combustion and expansion strokes and this is the results of fast flame propagation and destruction of tumble vertical to it.

The velocity vectors and streamlines in exhaust stroke are shown in figures 12.and 13., after combustion completion, in the exhaust stroke the tumble and angular momentum in Y direction increase very little. The tumble and angular momentum in X direction are shown in figures 14.and 15., as shown in figures, the tumble and angular momentum are negligible in all cycle except the start of combustion ,because with starting of ignition and releasing more energy at very small time, the momentum and tumble increase rapidly in three dimensional.

Figures 16. And 17. Show the in-cylinder bulk temperature counters at start and through of combustion. The operation condition of these figures is equivalence ratio (Phi=1.2) and compressed natural gas (CNG) fuel. Figure 18. Shows the bulk temperature variation versus crank angle for combustion of (CNG) at 2500rpm, compression ratio 9.13 and equivalence ratio 1.2. The temperature rise at ignition point shows start of combustion and will continue up to equilibrium point where the maximum temperature will obtain. Figure 19. Shows the variation of in-cylinder average pressure versus crank angle at different compression ratios. With increasing compression ratio, the peak pressure increases. Figure 20. shows the fuel concentration variation at the inlet of cylinder. The in-cylinder fuel value increases throughout the intake stroke up to around the top dead center. After this point, due to start of combustion the fuel concentration remain constant and with beginning of combustion, the oxidation of fuel starts and its value will consume.

The suddenly decreasing of methane mass indicates the ignition of it and shows the start of combustion and auto-ignition point of engine and this method can be used as criteria to detect the auto-ignition.

The variation of in-cylinder temperature and pressure with crank angle for compressed natural gas combustion are showed in figures 21 and 22 at different equivalence ratios. At very low equivalence ratio (Phi=0.4) and at this compression ratio the combustion not occurs but with increasing the equivalence ratio, the oxidation of fuel starts and the temperature and pressure are increasing.

The variation of OH, H and O concentrations with equivalence ratio are shown in Figures 23,24and 25. In the combustion of methane – oxygen mixture, the OH radical has important role than H radical and in the combustion of methane – air, the importance of H radical is much. This is shown in the figures 23 and 24 where, in the rich mixture the production of H radical is further than OH radical. Thus consideration of equilibrium concentrations for OH and H radicals is good approximation, because the production of OH radical is in a short time when the temperature is high enough. Due to the dependence of the reaction rates on temperature is much, the effect of initial temperature on auto-ignition is very important and with increasing the initial temperature the kinetic energy of species and number of collisions between species will increase rapidly and the combustion will start very earlier than other cases.

Figures 26 and 27 show the variation of CO and CO_2 concentration with time. The CO value increase rapidly at the start of combustion but after the combustion completion, the oxidation of CO will take more speed and its concentration will decrease and the CO_2 concentration will increase throughout oxidation of CO. Also, for stoichiometric condition, the CO2 will take its maximum value and has been decreased with increasing equivalence ratio.

The nitrogen oxides (NOx) are the important pollutants of internal combustion engines, the variation of nitrogen oxide (NO) is shown in figures.28 and 29. At the stoichiometric point, the concentrations will take maximum values and this is as a result of higher combustion temperature at this condition. When the mixture become richer, the oxygen concentration decreases and the maximum temperature and also the NOx concentrations will decrease and when the mixture become leaner, the maximum temperature decreases.

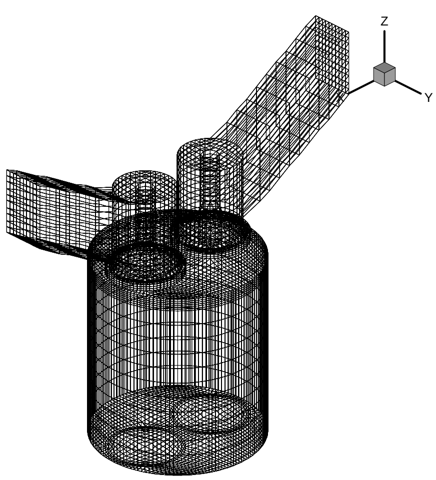

Figure 2. Mesh used in modeling

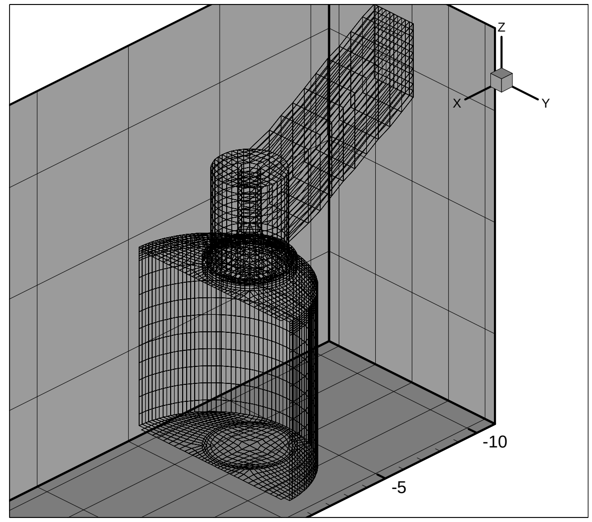

Figure 3. Mesh blanked at X=0.0

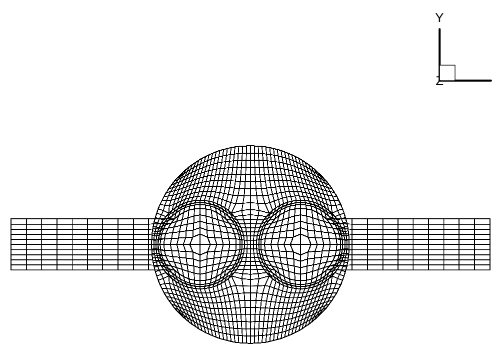

Figure 4. Mesh generated (xy view)

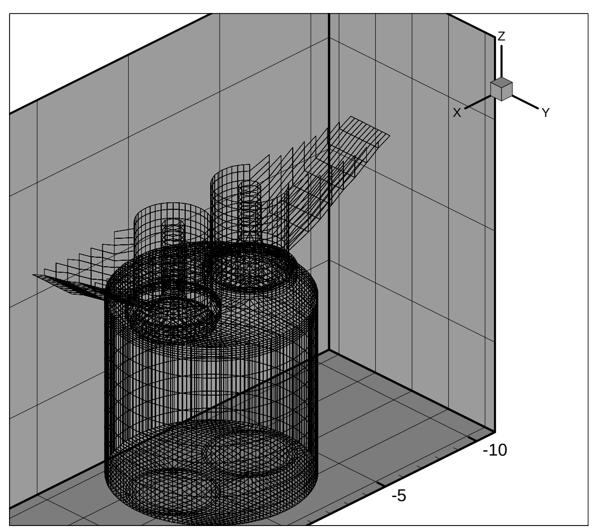

Figure 5. Mesh blanked at Z=10.0

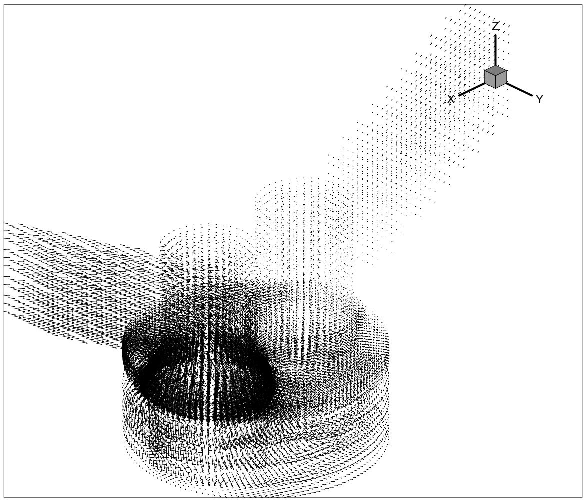

Figure 6. Velocity vectors at initial intake process.

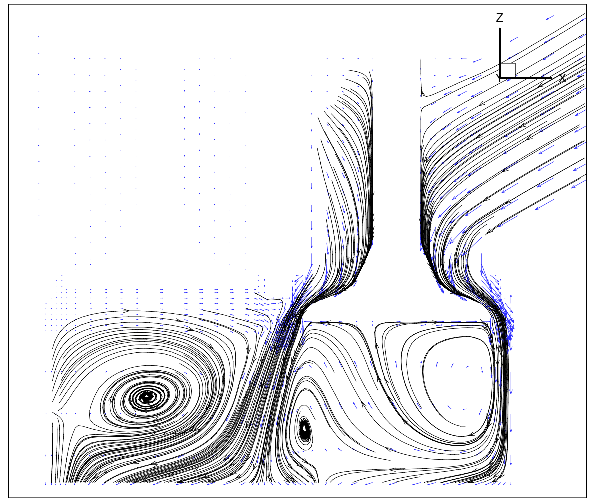

Figure7. Streamlines at the initial of intake.

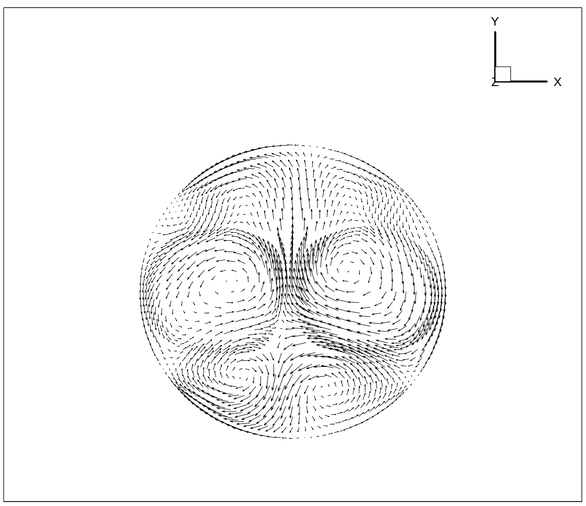

Figure 8. A section of velocity vectors.

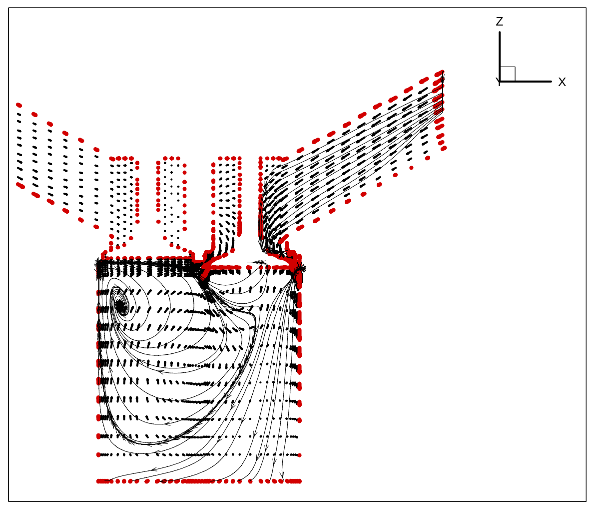

Figure 9. Streamlines at the end of intake process.

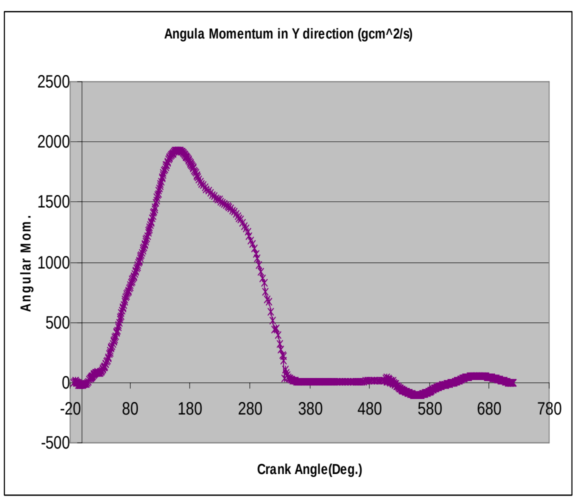

Figure 10. Angular momentum in Y direction.

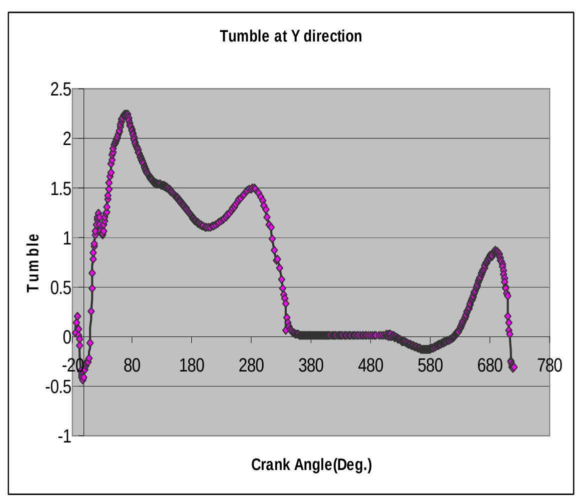

Figure 11. Tumble generation in Y direction.

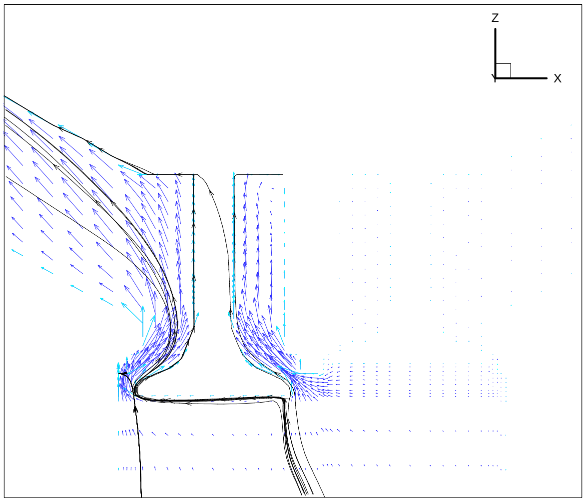

Figure 12. Velocity vectors and streamlines in the middle of exhaust processes.

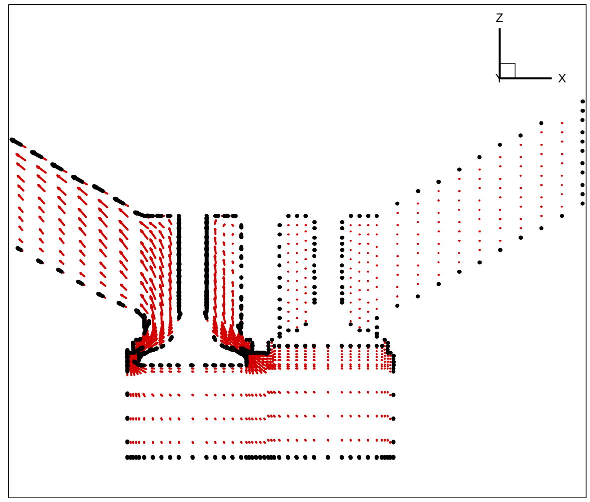

Figure 13. Velocity vectors in the end of exhaust processes.

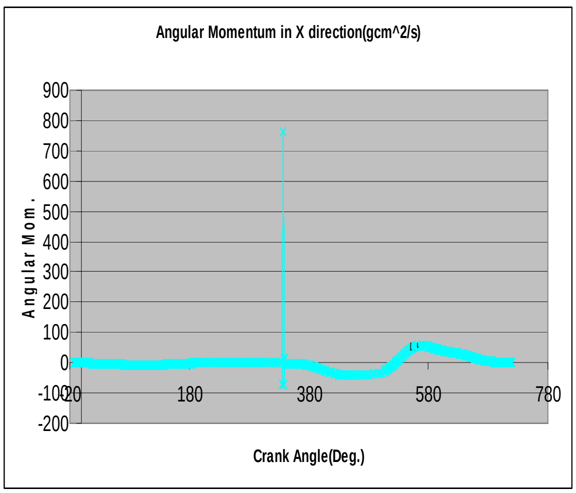

Figure 14. Angular momentum in X direction and in full cycle.

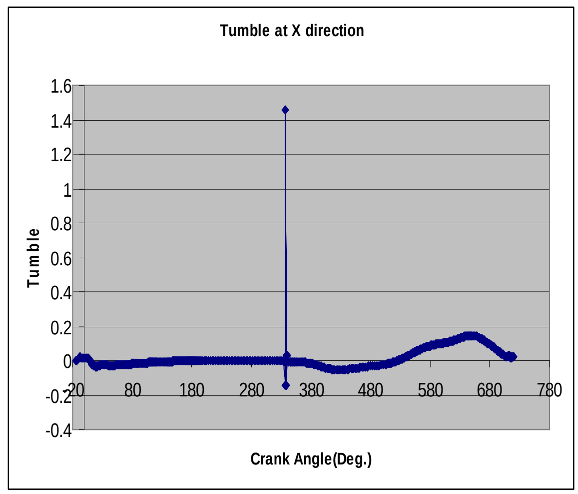

Figure 15. Tumble generation in X direction and in full cycle.

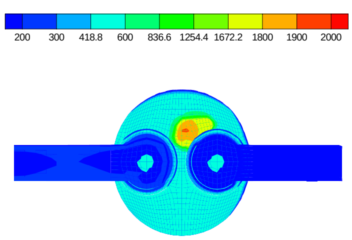

Figure 16. In-cylinder temperature counters at the start of combustion.

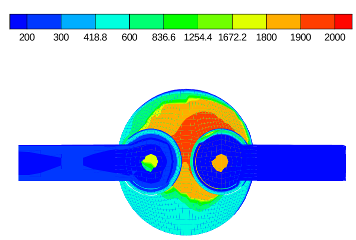

Figure 17. In-cylinder temperature counters through the combustion.

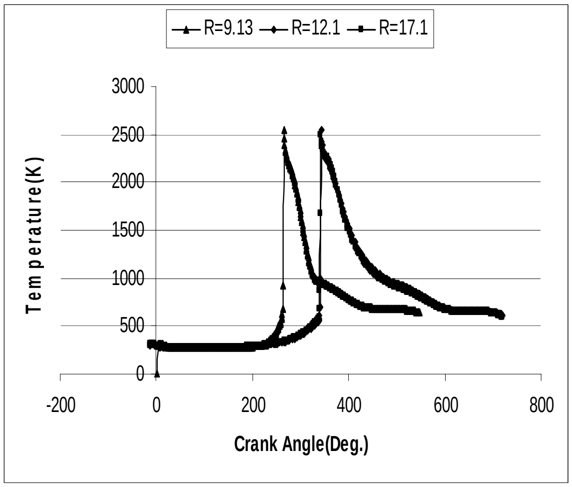

Figure 18. Variation of temperature Vs. Crank angle at equivalence ratio (φ=1.4).

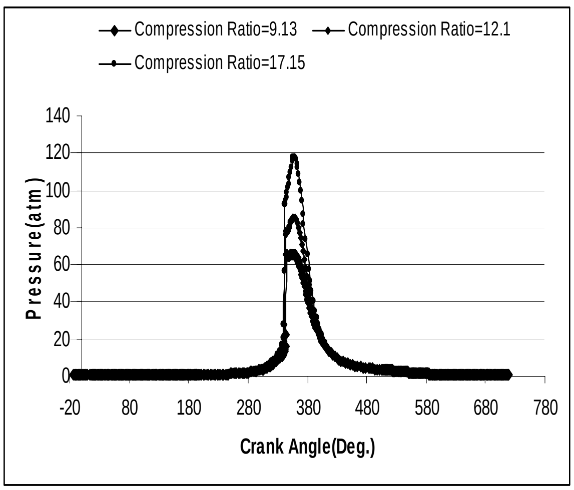

Figure 19. Variation of Pressure vs. Crank angle at equivalence ratio (φ=1.4).

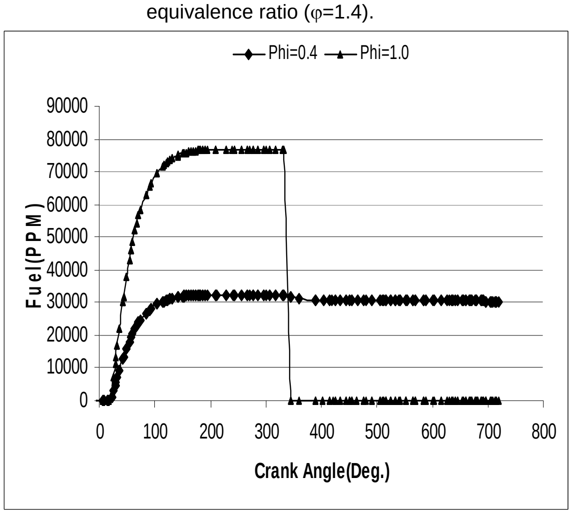

Figure 20. Variation of fuel (CH4) concentration vs. crank angle at different equivalence ratio.

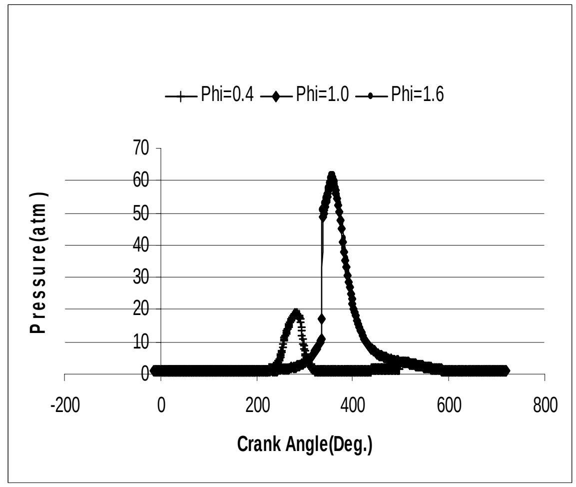

Figure 21. Variation of Pressure vs. Crank angle.

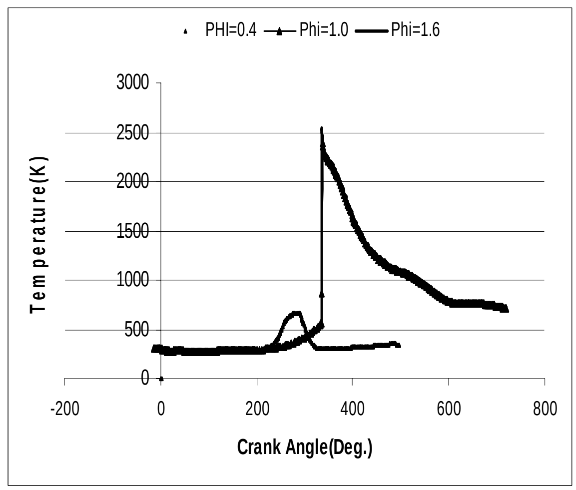

Figure 22. Variation of temperature Vs. Crank angle at different equivalence ratios.

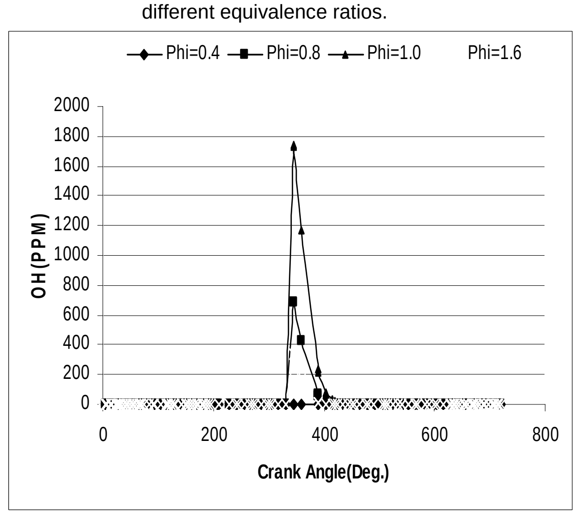

Figure 23. Variation of OH concentration with time.

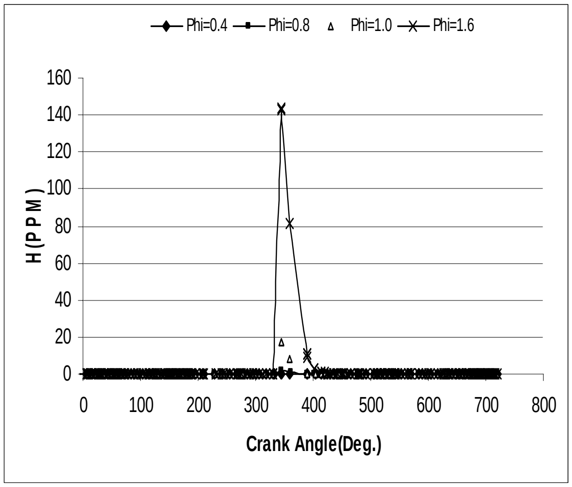

Figure 24. Variation of H concentration with time at different equivalence ratios.

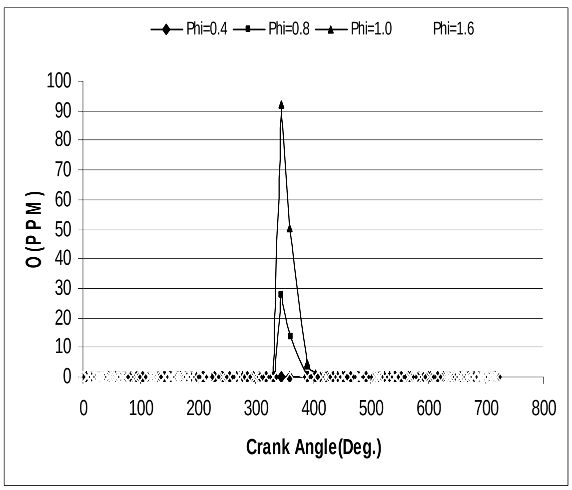

Figure 25. Variation of O concentration with time at different equivalence ratios.

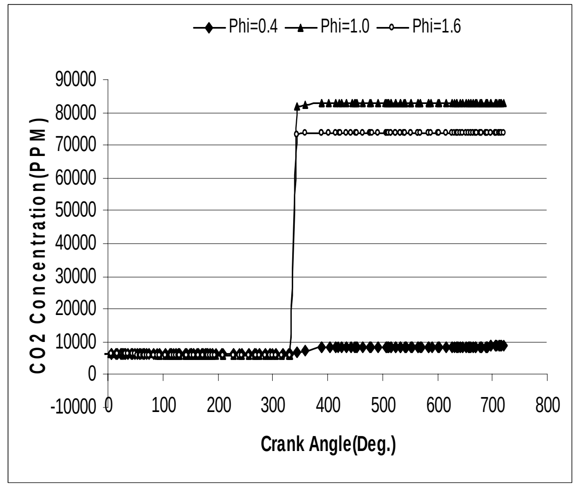

Figure 26. Variation of CO2 concentration with time at different equivalence ratios.

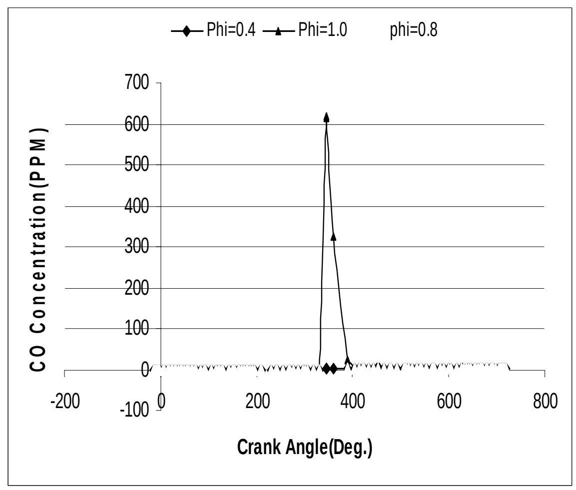

Figure. 27. Variation of CO concentration with time at different equivalence ratios.

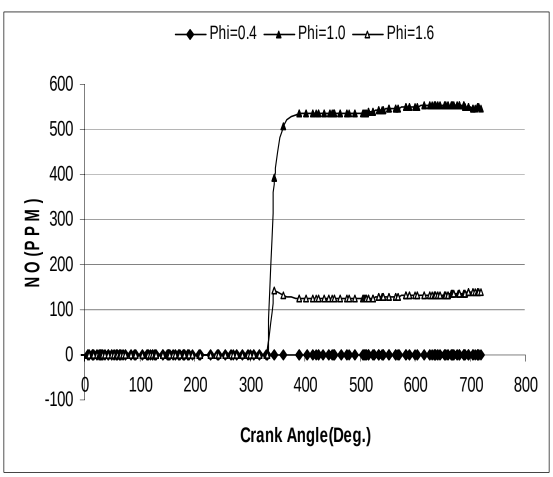

Figure 28. Variation of nitrogen oxide (NO) concentrations with time at different equivalence ratios.

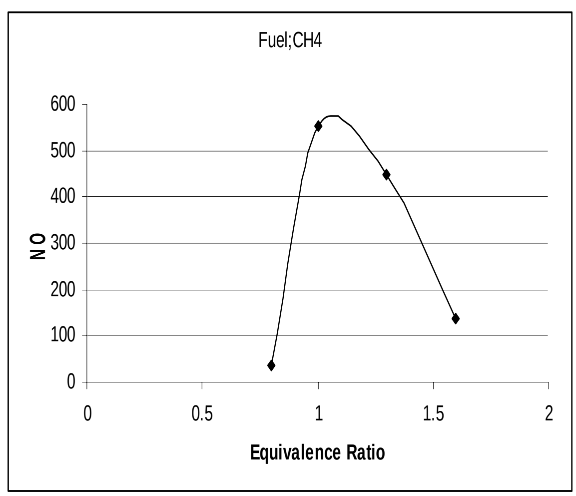

Figure 29. Variation of nitrogen oxide (NO) concentrations with equivalence

CONCLUSIONS

The performance and pollutants emissions from an internal combustion engine fueled with CNG (Natural Compressed Gas), has been studied with using multi-dimensional method. The variation of performance and emission parameters are agree with results proposed by author in earlier papers [28, 29, and 31] in general form. The prepared program has ability to study the effects of design and operating parameters on engine performance and pollutants emissions.

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