

# *A numerical investigation on the effects of using formaldehyde as an additive on the performance of an HCCI engine fueled with natural gas*

O. Jahanian<sup>\*1</sup>, S. A. Jazayeri<sup>2</sup>

<sup>1,2</sup>Department of Mechanical Engineering, K. N. Toosi University of Technology, Tehran, Iran

Received Date: 3 Apr.; 2011

Accepted: 3 Jun.; 2011

## **ABSTRACT**

In this paper, the performance of a natural gas HCCI engine is studied through a thermodynamic model including detailed chemical kinetics. It is shown that as hydroxyl radical has important effects on natural gas combustion, it is possible to quantify SOC with hydroxyl concentration variations. Meanwhile the influence of using formaldehyde as an additive on the engine characteristics has been investigated. Results show that it is possible to change the engine working limits using this additive. Lower autoignition temperature of formaldehyde causes advanced combustion in natural gas HCCI engine. In  $T_{IVC} = 410K$  case, adding 5% formaldehyde would lead to more than 10 CA advance in SOC. Furthermore, there is an optimum additive content for each operating condition, which leads to higher output work and power. It is also shown that the air/fuel mixture will ignite earlier using this additive so it is conceivable to reduce inlet mixture temperature resulting in better performance due to higher volumetric efficiency.

## **Keywords**

HCCI engine, start of combustion, thermodynamic modeling, natural gas, formaldehyde

## **1. Introduction**

Onishi et al. [1] introduced the concept of Homogenous Charge Compression Ignition (HCCI) for two-stroke internal combustion engines. They showed that compressing a homogenous mixture of air and fuel up to auto-ignition margin would effectively reduce fuel consumption and engine emissions. Noguchi et al. [2] developed this idea and emphasized the benefits at part load conditions. Najt et al [3] used this concept in four-stroke engines and finally Thring [4] named it as HCCI in 1989.

In HCCI engines, a homogenous premixed fuel/air mixture is sent into cylinder. The equivalence ratio of the mixture can change from 0.2 to 0.5 [5]. The mixture is compressed via piston

displacement up to autoignition point. The autoignition starts a rapid combustion phase that releases all the fuel heat in 5-15 CA. Heat release rate is controlled with highly diluted mixture using air or EGR. The HCCI concept affords the use of elevated compression ratios (approximately 17-20:1), unlike in spark ignition engines, which are susceptible to knock. The combination of lean burning and high compression ratios contributes to high thermal efficiencies that can approach 45% [6]. HCCI engines have demonstrated very low NO<sub>x</sub> emissions and PM, as well as high thermal efficiency at part loads. However, there are some difficulties in applying HCCI combustion to internal combustion engines. Ignition timing con-

<sup>\*</sup> Corresponding author: O. Jahanian (e-mail: o\_jahanian@alborz.kntu.ac.ir)  
Tel: +98-21-84063217; Fax: +98-21-88677274.

trol and homogenous mixture preparation are the main difficulties of HCCI engines [7].

Engine simulation studies have been used to explore the HCCI concept. Simulation can be held under several methods. These methods include single and multi-zone thermodynamic models and CFD codes. Ref [8] represents a brief description and comparisons for these methods.

Natural gas is well suited to the HCCI combustion concept because of minimal mixture preparation requirements and chemical stability. Natural gas exhibits a relatively simple molecular structure, which reacts to yield far less intermediate compounds as well as a low carbon to hydrogen ratio (1:3.87) that results in reduced harmful exhaust gas emissions. Its high ignition resistance when coupled with lean fuel/air mixtures affords the use of elevated compression ratios without pre-ignition of the charge [6].

Many compounds such as propane, butane, hydrogen peroxide, and formaldehyde are used as an additive in natural gas fueled engines. Formaldehyde is one the most common additives which has been utilized in many researches [9-14].

Kentaro et al. [9] showed that formaldehyde strongly affects production/consumption rate of hydroxyl radicals and therefore it can be used to control the combustion of an HCCI engine. Numerical results of Morsy et al. [10, 11] have indicated the effects of using formaldehyde on advanced autoignition in natural gas fueled HCCI engines. Chen et al. [12] figured out formaldehyde would reduce the exothermicity of low temperature combustion reaction of dimethyl ether and therefore leads to advanced combustion.

This paper utilized a single zone zero dimensional model to investigate the effects of using formaldehyde as an additive on performance of a single cylinder Caterpillar 3500 engine running under HCCI mode.

High computational speed, appropriate precision for calculating parameters such as SOC and in cylinder temperature/pressure trends are the main reasons of using this model. The effects of formaldehyde on temperature and pressure trend of incylinder mixture, start of combustion and engine performance characteristics is described in detail. The studies have been done for different initial temperatures of inlet air/fuel mixture.

## **2. Formaldehyde**

Formaldehyde is the simplest aldehyde in organic compounds category with chemical formula  $\text{CH}_2\text{O}$ . It is one of the intermediate species of natural gas combustion mechanism. It can increase the combustion reaction rates when used as an additive.

Table 1 shows the physical properties of formaldehyde in comparison to major gases in natural gas composition. Formaldehyde is categorized as a hazardous material and it should be used under tight legislations. According to EPA regulations [15], the allowed quantity of formaldehyde in air is 16ppb.

## **3. Thermodynamic modeling of HCCI engine**

### **3.1. Model assumptions**

A zero dimensional single zone model including detailed chemical kinetics has been developed for thermodynamic modeling of an HCCI engine. The main assumptions of the model can be expressed as:

- The HCCI engine is single-cylinder four-stroke.
- Only the closed cycle from IVC to EVO has been considered in the model.
- The whole cylinder is assumed as a single zone with uniform temperature and pressure.
- The incylinder mixture is treated as ideal gas.
- Blow-by is neglected.
- The mixture at IVC is thoroughly homogenous.
- Modified Woschni model is used to evaluate the heat transfer to cylinder wall.

### **3.2. Natural gas combustion mechanism**

GRI Mech. 3.0 [17] detailed chemical kinetics including 325 primary reactions with 53 chemical species is used for appropriate study on the combustion characteristics of the engine. The GRI Mech. 3.0 mechanism includes extended Zeldovich mechanism and is suitable for prediction  $\text{NO}_x$  emissions.

Table 1. Formaldehyde properties in comparison to major gases in natural gas composition [16]

Properties	Formaldehyde	Methane	Ethane	Propane
Chemical Structure	CH <sub>2</sub> O	CH <sub>4</sub>	C <sub>2</sub> H <sub>6</sub>	C <sub>3</sub> H <sub>8</sub>
Molar Weight (g/mole)	30	16	30	44
Autoignition Tem. (K)	430	595	515	470
Explosive Limits (%)	7-73	5-15	3-12.5	2-9.5

### 3.3. Programming

The model has been developed in MATLAB<sup>®</sup> programming environment using CANTERA<sup>®</sup> module for combustion modeling.

The model is stand-alone and has the ability to use CHEMKIN<sup>®</sup> mechanism library. It can be easily joined to other codes and the results can be used as the input of control systems.

### 3.4. Implementation of Energy and Mass Conservation Equations

In the developed zero-dimensional model, the whole combustion chamber is considered as a control volume. Energy and mass conservation equations should be solved simultaneously for this system.

The energy conservation equation for this control volume can be described as,

$$\delta Q - \delta W = dU \quad (1)$$

Equation (1) can be rewritten for the mixture of several chemical species as,

$$\delta Q - PdV = mdu + m \sum_{i=1}^{N_s} u_i dy_i \quad (2)$$

As  $Q$  is only due to heat transfer to cylinder wall and the mixture is a perfect gas,

$$\frac{dq}{dt} - P \frac{dV}{dt} = mC_v \frac{dT}{dt} + m \sum_{i=1}^{N_s} u_i \frac{dy_i}{dt} \quad (3)$$

By separating the temperature terms, the first differential equation of the model can be obtained,

$$\frac{dT}{dt} = \frac{\frac{1}{V} \left( \frac{dq}{dt} - P \frac{dV}{dt} \right) - \rho \sum_{i=1}^{N_s} u_i \frac{dy_i}{dt}}{\rho C_v} \quad (4)$$

This equation describes that the in-cylinder temperature variations, originate from two sources:

- Energy transfer through control volume border
- Variation in chemical composition of the system

The mass conservation in chemical reacting systems is defined as the conservation of chemical elements. The rate of mole fraction variation of chemical species can be computed as,

$$\frac{dy_i}{dt} = \frac{M_i \omega_i}{\rho} \quad (5)$$

Equation (5) should be written for every chemical component and this set of equations must be solved simultaneously with equation (4).

A detailed chemical kinetics mechanism is needed to determine the production/consumption rate of each chemical component ( $\omega_i$ ).

Now, there is a need for another differential equation to enclose the differential equations system. This equation defines the rate of variations in combustion chamber [18] via a slider-crank formula,

$$V = V_c \left( 1 + \frac{r_c - 1}{2} \left( R + 1 - \cos \theta - \sqrt{R^2 - \sin^2 \theta} \right) \right) \quad (6)$$

### 3.5. Chemical kinetics

The Mass Action rule [19] explains the reaction rate for each direction of an equilibrium reaction depends on reactants' concentration and their stoichiometric coefficients. Therefore, the reaction rate is,

$$RR = k_f [A]^a [B]^b - k_b [C]^c \quad (7)$$

The rate constant  $k$  is determined by Arrhenius relation in equation (8).

$$k = A_{Ar} T^\beta \exp \left( \frac{-E_a}{R_u T} \right) \quad (8)$$

Each chemical reaction mechanism consists some primary reactions which are either simple or with a third body. A simple primary reaction can be assumed as,

$$\sum_{j=1}^{N_s} \nu'_{j,i} S_j \square \sum_{j=1}^{N_s} \nu''_{j,i} S_j \quad i = 1, 2, \dots, N_R \quad (9)$$

For each simple primary reaction, the reaction rate equation turns to,

$$RR_i = k_{f,i} \prod_{j=1}^{N_s} [S_j]^{\nu'_{j,i}} - k_{b,i} \prod_{j=1}^{N_s} [S_j]^{\nu''_{j,i}} \quad (10)$$

Some primary reactions need a third body to be done.

As the concentration of the third body affects the reaction rate, it differs from equation (10) and should be written as,

$$\sum_{j=1}^{N_s} \nu'_{j,i} S_j + TB \square \sum_{j=1}^{N_s} \nu''_{j,i} S_j + TB \quad (11)$$

The third body concentration includes the concentrations of all species due to their enhance factor. Therefore, the reaction rate for these types of primary reactions is,

$$RR_i = \left( \sum_{j=1}^{N_s} a_{j,i} [TB_j] \right) \times \left( k_{f,i} \prod_{j=1}^{N_s} [S_j]^{\nu'_{j,i}} - k_{b,i} \prod_{j=1}^{N_s} [S_j]^{\nu''_{j,i}} \right) \quad (12)$$

The coefficients can be obtained from different sources like NASA polynomials [20]. So the production/consumption rate of each chemical component can be calculated as,

$$\dot{\omega}_i = \sum_{j=1}^{N_R} RR_j (\nu'_{i,j} - \nu''_{i,j}) \quad (13)$$

### 3.6. Heat transfer model

For defining  $dq/dt$ , it is common to use Woschni heat transfer model for traditional internal combustion engines, but due to the rapid combustion period of HCCI engines, a modified relation [21] has been used in this paper.

This modified model describes,

$$\frac{dq}{dt} = hA(T - T_w) \quad (14)$$

where the convection heat transfer coefficient is,

$$h = 129.8L^{-0.2} P^{0.8} T^{-0.73} (2.28S_p + f(P))^{0.8} \quad (15)$$

$$f(P) = 3.34 \times 10^{-4} \frac{V_d T_r}{P_r V_r} (P - P_{mot})$$

### 3.7. Model validation

The developed model has been validated with experimental data for two types of engines in different operating conditions. The procedure has been presented in authors' previous works [22-24]. Comparisons show the appropriate accuracy of the model to predict the operational conditions of an HCCI engine. Similar to all zero dimensional models, the peak cylinder pressure/temperature is higher than the experimental results, and occur earlier. This is because of:

- The homogeneity of combustion chamber is the main assumption of single zone models. But in real cases, there are some inhomogeneities in fuel/air mixture at IVC and also during the engine strokes, the near-wall areas has lower temperature because of heat transfer to cylinder wall.
- Single zone models, neglect blow-by, and the unburnt amount of fuel in crevices so the pressure is over predicted in the simulation.

Although single zone models are widely used because of their low computational requirements, accurate prediction of SOC and NO<sub>x</sub> [6, 8, 10], but they are not able to predict carbon monoxide, UHC and PM emissions due to neglecting the crevices and cold regions near cylinder wall.

### 4. Defining start of combustion

Start of Combustion (SOC) is a leading factor affecting on HCCI engine performance. Several methods are suggested for defining SOC in HCCI engines. The most common methods can be categorized as,

- Defining a temperature threshold
- Calculation the third derivation of pressure trace due to crank angle
- Knock Integral Method
- Chemical kinetics models

Defining a temperature threshold for SOC [25] includes a lot of uncertainties. The threshold temperature of combustion depends on numerous parameters, which make it difficult to use. In the second method [26], the numerical value of

$d^3P/d\theta^3$  at each crank angle is calculated during compression stroke and SOC would be defined as this parameter reaches a specified value.

$$\left. \frac{d^3P}{d\theta^3} \right|_{SOC} = 0.25 \quad (16)$$

In Knock Integral Method (KIM) [27], an integral function of temperature, pressure, equivalence ratio, is defined. This function is calculated during compression stroke and the crank angle that the integral reaches the value of 1, is defined as SOC. Constants of this function depend on engine geometry and fuel type. There is no need to chemical kinetics for these methods.

In chemical kinetics methods, the variations in the concentration of specified species is studied and SOC is defined due to the mole fraction of a specified radical depending on the fuel type. Some of these models utilize reduced chemical kinetics like Shell [28] and Hu and Ceck [29]; others use detailed chemical kinetics [6]. These methods are fully dependent on fuel type and the intermediate radicals produced in combustion mechanism. As this study uses natural gas as fuel, the maximum derivation of hydroxyl radical production rate due to crank angle is considered as SOC. This method is thoroughly described in the results and discussion section for natural gas fuel.

### 5. Defining the equivalence ratio

The equivalence ratio of a fuel/air mixture is concerned to the fuel composition. In this paper, the composition of natural gas is considered as the major composition used in Iran including 89% methane, 4.5% ethane, 1.5% propane, 4.75% nitrogen, and 0.25% carbon dioxide (volume fraction) [30]. The amount of adding formaldehyde is also described as volume fraction of total fuel. If  $x_f$  stands for volume fraction of formaldehyde, the stoichiometric air/fuel ratio can be shown as,

$$(A/F)_{st} = 9.58 - 4.82x_f \quad (17)$$

It should be mentioned that using formaldehyde as an additive causes the fuel be categorized as oxygenated fuel so the atom valence method should be used to evaluate the equivalence ratio

[31]. In this method, the valence of carbon, hydrogen, oxygen, and nitrogen atoms are +4, +1, -2 and 0. The real equivalence ratio is the ratio between total positive and negative valences.

$$\phi = \frac{\sum V^+}{\sum V^-} = \frac{n_c \times 4 + n_H}{n_o \times 2} \quad (18)$$

### 6. Results and discussions

The developed code has been run several times to investigate the influence of different parameters on operational characteristics of single cylinder Caterpillar 3500 engine running in HCCI mode. The engine specifications are shown in table 2.

First, the influence of inlet air/fuel temperature without adding formaldehyde has been studied. Figures 1 and 2 show the pressure and temperature trends for three different temperatures at IVC. As seen in the figures, there is no combustion in the  $T_{IVC} = 390K$  case because the mixture pressure and temperature do not reach the autoignition limit. In such a case, it is usually noted that the engine is out of its operating range. In  $T_{IVC} = 410K$  case, the combustion occurs slightly after TDC. By increasing the inlet temperature to  $T_{IVC} = 430K$ , the combustion occurs before TDC and the maximum value of pressure and temperature rises. It can be seen that the combustion phenomena is highly concerned to initial temperature and it can be used as a control parameter. Inlet air preheating and using hot EGR are some available ways to set the initial temperature of the mixture. In other hands, it should be mentioned that increasing inlet mixture

Table 2. Caterpillar 3500 engine Specifications

Properties	Value
Bore (mm)	170
Stroke (mm)	190
Rod length (mm)	350
Compression ratio	17
IVC (ABDC)	20
EVO (BBDC)	40
Speed (rpm)	1500
Cylinder wall temperature (K)	400

temperature would lead to lower engine volumetric efficiency and amount of fuel entering the cylinder.

Methane is the main compound in the natural gas composition. The low temperature oxidation of methane starts via these primary reactions,



The variation in the concentrations of hydroperoxy ( $HO_2$ ) and hydrogen ( $H$ ) radicals are shown in fig.3 for combustion ( $T_{IVC} = 410K$ ) and no combustion ( $T_{IVC} = 390K$ ) cases.

In combustion case, the concentrations of these radicals rapidly rise but in no combustion case, this increase is extremely slight and because of temperature raise due to incylinder volume changes.

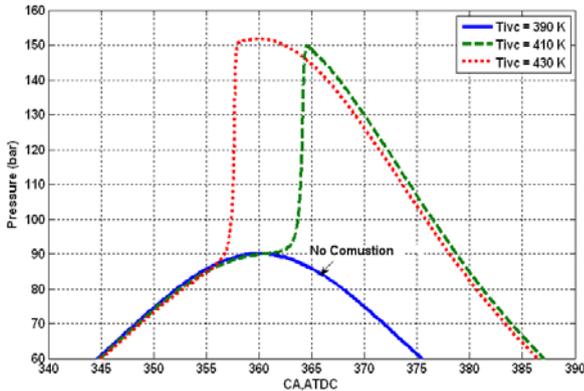


Fig. 1: Incylinder pressure variation for three different inlet temperatures at IVC

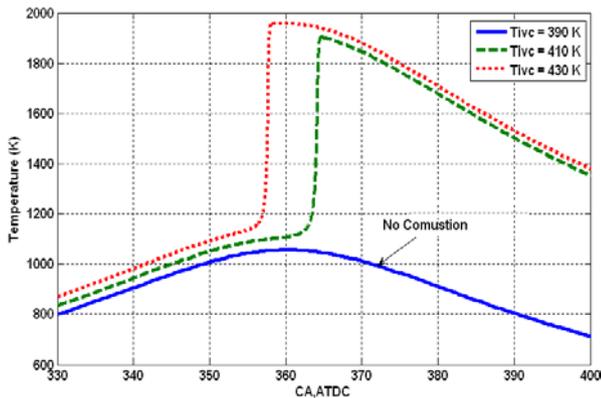


Fig. 2: Incylinder temperature variation for three different inlet temperatures at IVC

Hydroperoxy and hydrogen radicals quickly attend the propagating reactions and advance the chain reactions by producing hydroxyl radical ( $OH$ ) and hydrogen peroxide ( $H_2O_2$ ).



The hydrogen peroxide also decomposes to hydroxyl radicals.



This reaction produces high amounts of hydroxyl radicals. The reaction between hydroxyl radical and fuel molecule is highly exothermic. The radical concentration variation near combustion point is illustrated in fig.4.

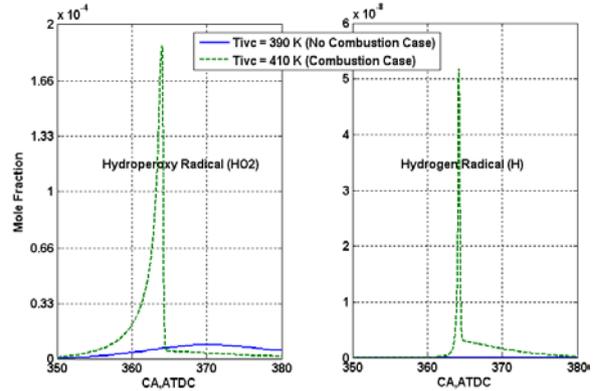


Fig. 3: Variations in hydroperoxy and hydrogen radicals for combustion and no combustion cases

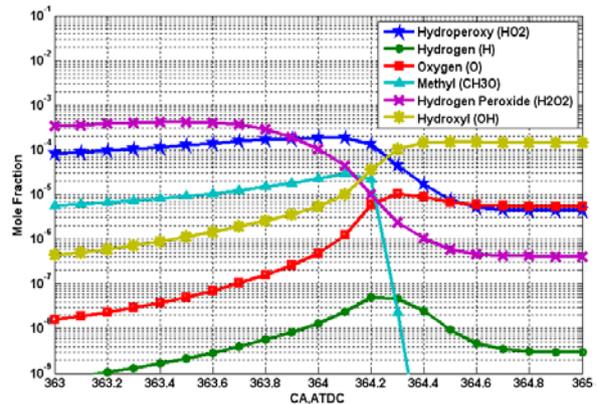


Fig. 4: Concentrations of important radicals near TDC

Considering this issue, SOC can be defined as the crank angle in which hydroxyl radical concentration shows a rapid raise. This could be quantified by the maximum value of hydroxyl radical trend slope. A comparison between this detailed chemical kinetics model and the third derivation of pressure trace method for defining SOC is presented in table 3. The results show a good agreement between these two common methods.

Formaldehyde has a lower autoignition temperature in comparison to other natural gas components, therefore it is logical that using formaldehyde as an additive would advance the HCCI combustion. Fig. 5 shows the effects of adding 2%, 5%, and 10% formaldehyde on the no combustion case ( $T_{IVC} = 390K$ ).

Results show that even adding 1% formaldehyde to natural gas at  $T_{IVC} = 390K$  will lead to combustion whereas the natural gas would not individually ignite in this condition. With 1% additive, the combustion starts at 363.9 CA, which does not seem appropriate but adding more formaldehyde would end in more advanced combustion. As seen in the figure, SOC will occur at 355.5 CA by adding 10% formaldehyde which is 8.4 CA earlier in comparison to 1% additive usage.

Increasing inlet mixture temperature is a common path to achieve autoignition in HCCI engines but increasing inlet temperature would lead to lower volumetric efficiency and less amount of entering fuel. In the presented case, natural gas HCCI engine would not go under operation condition at  $T_{IVC} = 390K$  and should have higher inlet temperature to ignite but adding formaldehyde has changed this operation limit and the engine would be run with a lower inlet temperature. Lowering inlet mixture temperature would significantly lead to lower NOx emissions.

For a detailed study on the effects of using formaldehyde as an additive on the performance of an HCCI engine, the engine major parameters such as gross values of indicated work and power, mean effective pressure, specific fuel consumption, SOC and NOx emissions have been considered.

The amount of additive was held in 1-5% range according to previous experiments [10, 11].

Fig. 6 shows the variations in these parameters for  $T_{IVC} = 390K$  case.

Increasing formaldehyde from 1% to 5% causes SOC changes from 363.9 CA to 357.4 CA. On the other hand, NOx emission will be doubled because of higher incylinder maximum temperature and extended high temperature duration in the combustion stroke. This is usually called thermal NOx.

Table 3. Comparison between SOC predicted by two different methods

Case	Predicted SOC (CA, ATDC)		Absolute Difference
	Method 1	Method 2	
TIVC = 410 K	364.2	364.1	0.1
TIVC = 430 K	357.7	375.5	0.2

Method 1 : Hydroxyl Concentration Variations  
Method 2 : 3rd Derivation of Pressure Trace

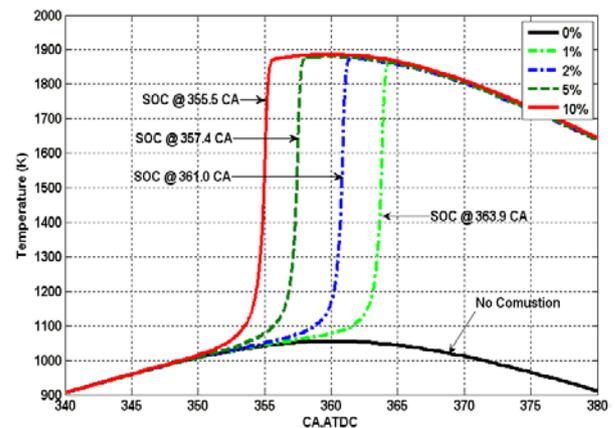


Fig. 5: The effects of using formaldehyde on temperature trend

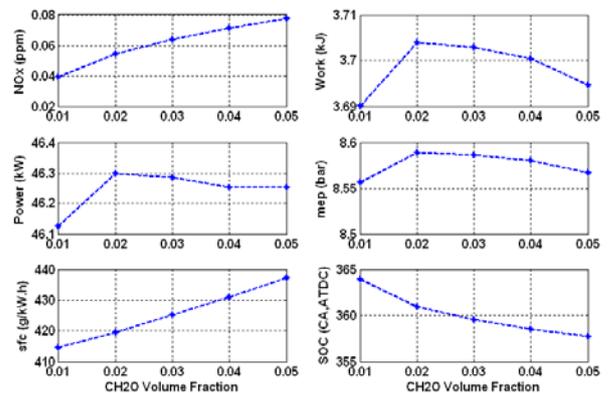


Fig. 6: The effects of using formaldehyde on engine performance ( $T_{IVC}=390K$ )

Comparing engine power and output work in different cases shows that these parameters rise slowly by increasing additive amount up to a maximum value then a reverse trend is observable.

The maximum value obtained with 2% formaldehyde. Although specific fuel consumption linearly increases by adding more formaldehyde but it should be mentioned that natural gas with no additive would not ignite at this condition and adding formaldehyde causes the engine to work at lower temperature that extremely decreases NOx amount and increases engine volumetric efficiency in comparison to  $T_{IVC} = 410K$  case.

The same study has been repeated for  $T_{IVC} = 410K$  case. Results are shown in fig.7. The same trends are seen here. The optimum performance at this condition would be obtained by 1% formaldehyde addition.

In  $T_{IVC} = 410K$  case with no additive, the output power is about 43.6 kW with 0.058 ppm NOx emission but using 1% additive in  $T_{IVC} = 390K$  case would lead to 46.1 kW power with 0.039 ppm NOx emission.

Adding 2% formaldehyde in this case would increase the output power to 46.3 kW with 0.054 ppm NOx (almost the same as  $T_{IVC} = 410K$  case with no additive). It is obvious that the effect of using additive in lowering the initial temperature would lead to better engine operating condition considering output power and NOx emission.

A comparison between the optimum conditions in figures 6 and 7 studies is shown in table 4. In this table, case I represents the 2% formaldehyde addition at  $T_{IVC} = 390K$  condition and case II is 1 % formaldehyde addition at  $T_{IVC} = 410K$  condition. The last column shows relative value of case I in respect of case II.

Although there is a retarded combustion in case I, but gross indicated power and work is about 6% higher in comparison to case II whereas fuel consumption is just 1% more.

Lower temperature of inlet mixture in case I, leads in higher volumetric efficiency and higher amount of inlet fuel, which directly affects engine power. Adding 2% formaldehyde changes the lower operating limit of the engine and it can be run at  $T_{IVC} = 390K$  condition. on the other

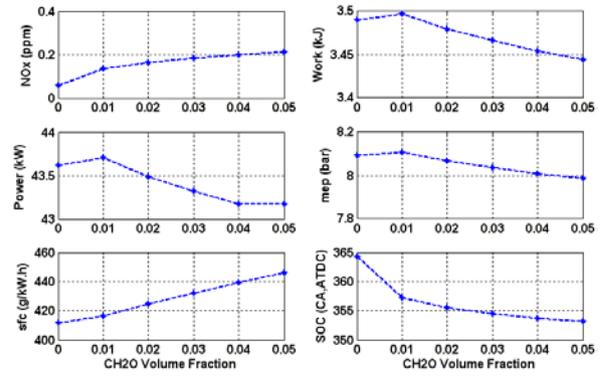


Fig. 7: The effects of using formaldehyde on engine performance ( $T_{IVC}=410K$ )

Table 4. Operational characteristics of HCCI engine in two optimum cases of using additive

Properties	Case I	Case II	ratio
<i>SOC (CA, ATDC)</i>	361.0	357.3	+ 3.7 CA
<i>Gross Indicated Work (kJ)</i>	3.70	3.50	+ 5.71%
<i>Gross Indicated Power (kW)</i>	46.30	43.71	+ 5.93%
<i>mep (bar)</i>	8.59	8.11	+ 5.92%
<i>sfc (J/kW.h)</i>	419.62	416.20	+ 0.82%
<i>NOx (ppm)</i>	0.054	0.137	- 60.58%

hand, decreasing incylinder temperature extremely decreases NOx emissions.

The table shows that amount of NOx emissions in case I, is about 60% lower than that in case II.

It should be noted that almost the total amount of formaldehyde added to the fuel would burn during combustion stroke. In  $T_{IVC} = 390K$  case with 5% additive, the mass fraction of formaldehyde at EVO is in the order of  $10^{-14}$  and in  $T_{IVC} = 410K$  case with the same percent; the value turns to  $10^{-17}$ .

These mass fractions are lower that permitted amount ( $1.6 \times 10^{-5}$ ). The same results were previously presented in different studies [12-14]. Indeed, there should be a special consideration about the technologies used for formaldehyde addition and control strategies to avoid additive leakage.

## 7. Summary and conclusions

The results of this study can be summarized as below:

- The developed single zone zero dimensional model can predict SOC in HCCI engine with appropriate uncertainty and it is suitable for comparative on studies.
- The temperature of inlet mixture strongly affects the combustion of HCCI engine. Decreasing initial temperature would cause the engine to go out of operating range and increasing initial temperature would result in more advanced combustion.
- Hydroxyl radical has important effects on natural gas combustion and it is possible to quantify SOC with hydroxyl concentration variations.
- Lower autoignition temperature of formaldehyde causes advance combustion in natural gas HCCI engine. In  $T_{IVC} = 410K$  case, adding 5% formaldehyde would lead to more than 10 CA advance in SOC.
- It is possible to change HCCI operating range by adding formaldehyde. In the specified HCCI engine, the mixture would not ignite at  $T_{IVC} = 390K$  but even adding 1% formaldehyde would result in mixture combustion.
- There is an optimum value of additive for each operating condition, which results in higher engine power. This optimum value is 2% for  $T_{IVC} = 390K$  case and 1% for  $T_{IVC} = 410K$  case.
- As the main source of NO<sub>x</sub> in HCCI engine is concerned to thermal NO<sub>x</sub>, adding formaldehyde to natural gas would increase engine NO<sub>x</sub> emissions because the maximum cylinder temperature and high temperature duration would increase by adding formaldehyde.

## 8. Nomenclature

A	Area
a	Enhance factor of third body
$A_{Ar}$	Arrhenius coefficient
$C_v$	Specific heat in constant volume
$E_a$	Activation energy
h	Convection heat transfer coefficient

i,k	Counter
$k_b$	Backward reaction rate constant
$k_f$	Forward reaction rate constant
L	Instantaneous height of combustion chamber
$M_i$	Molar weight of component i
m	Mass
$N_R$	Number of reactions
$N_S$	Number of species
P	Pressure
$P_m$	Motoring pressure
$P_r$	Reference pressure at IVC
Q	Heat
q	Heat transfer to cylinder wall
R	Rod length/ cranks radius ratio
$R_u$	Universal gas constant
$r_c$	Compression ratio
$RR_b$	Backward reaction rate
$RR_f$	Forward reaction rate
$RR_i$	Rate of reaction i
$S_i$	Component i
$S_p$	Average piston speed
T	Temperature
$T_r$	Reference temperature at IVC
$T_w$	Cylinder wall temperature
TB	Third body
U	Internal energy
u	Specific internal energy
$u_i$	Specific internal energy of component i
V	Volume
$V_c$	Clearance volume
$V_d$	Displacement volume
$V_r$	Reference volume at IVC
w	Work
$y_i$	Mole fraction of component i

### Greek Symbol

$\nu'_{i,k}, \nu''_{i,k}$	Stoichiometric coefficient of component i in forward/backward direction of reaction k
$\beta$	Arrhenius coefficient

$\phi$	Equivalence ratio
$\theta$	Crank angle
$\rho$	Density
$\omega_i$	Production/consumption rate of component i

#### Abbreviations

ATDC	After Top Dead Center
CA	Crank angle
CFD	Computational Fluid Dynamics
EGR	Exhaust Gas Residual
EVO	Exhaust Valve Opening
HCCI	Homogenous Charge Compression Ignition
IVC	Inlet Valve Closing
NOx	Oxides of Nitrogen
PM	Particulate Matter
SOC	Start of Combustion
UHC	Unburned Hydrocarbons

#### References

- [1] S. Onishi, S. Hong Jo, K. Shoda, S. Kato, Active Thermo-Atmosphere Combustion (ATAC) – A New Combustion Process for Internal Combustion Engines, SAE Paper No. 790501, 1979.
- [2] M. Noguchi, T. Tanaka, Y. Takeuchi, A Study on Gasoline Engine Combustion by Observation of Intermediate Reactive Products during Combustion, SAE Paper No. 790840, 1979.
- [3] P.M. Najt, D.E. Foster, Compression-Ignited Homogenous Charge Combustion, SAE Paper No. 830264, 1983.
- [4] R.H. Thring, Homogenous Charge Compression-Ignition (HCCI) Engines, SAE Paper No. 892068, 1989.
- [5] T.W. Ryan, T. Callahan, Homogenous Charge Compression Ignition of Diesel Fuel, SAE Paper No. 961160, 1996.
- [6] S.B. Fiveland, M. Christensen, B. Johansson, J. Hiltner, F. Mauss, D.N. Assanis, Experimental and Simulated Results Detailing the Sensitivity of natural Gas HCCI Engines to Fuel Composition, SAE Paper No. 2001-01-3609, 2001.
- [7] R.H. Stanglmaier, C.E. Roberts, Homogenous Charge Compression Ignition (HCCI): Benefits, Compromises, and Future Engine Applications, SAE Paper No. 1999-01-3682, 1999.
- [8] Z. Wang, S.J. Shuai, J.X. Wang, G.H. Tian, X.L. An, Modeling of HCCI Combustion: From 0D to 3D, SAE Paper No. 2006-01-1364, 2006.
- [9] M. Kentaro, Y. Yoshiyuki, K. Mitsuru, Control of HCCI Combustion by Adding Formaldehyde, Nihon Kikai Gakkai Nenji Taikai Koen Ronbunshu 7 (2004) 203-204. (in Japanese)
- [10] M.H. Morsy, S.H. Chung, Fundamental Study on the Influence of Additives on Ignition Control of Natural Gas HCCI Engine, JSAE Paper No. 20056029, 2005.
- [11] M.H. Morsy, Ignition Control of methane Fueled Homogenous Charge Compression Ignition Engines Using Additives, Fuel 86 (2007) 533-540.
- [12] Z. Chen, M. Konno, K. Miki, Computational and Experimental Study on the Influence of Formaldehyde on HCCI Combustion Fueled with Dimethyl Ether, SAE Paper No. 2003-01-1826, 2003.
- [13] H. Yamada, K. Suzuki, H. Sakanashi, N. Choi, A. Tezaki, Kinetic measurements in homogeneous charge compression of dimethyl ether: role of intermediate formaldehyde controlling chain branching in the low-temperature oxidation mechanism, Combust. Flame 140 (2005) 24–33.
- [14] Y. Yamaya, M. Furutani, Y. Ohta, Advanced/retarded criterion on ignition of fuel/air mixtures with formaldehyde doping, The 6th international symposium on diagnostics and modeling of combustion in internal combustion engines COMODIA, 2004.
- [15] <http://www.epa.gov/iris/subst/0419.htm>
- [16] R.C. Weast, CRC Handbook of Chemistry and Physics, 62nd ed., FL: CRC Press, Boca Raton, 1981.
- [17] G.P. Smith, D.M. Golden, M. Frenklach, N.W. Moriarty, B. Eiteneer, M. Goldenberg, C.T. Bowman, R.K. Hanson S. Song, W.C. Gardiner Jr., V.V. Lissianski, Z. Qin, GRI 3.0 Mechanism, Gas Research Institute ([http://www.me.berkeley.edu/gri\\_mech](http://www.me.berkeley.edu/gri_mech)).
- [18] J.B. Heywood, Internal Combustion Engine Fundamentals, 1st ed., McGraw-Hill Book Company, Singapore, 1988.
- [19] K.K. Kuo, Principles of Combustion, 1st ed., John Wiley & Sons, Inc., Singapore, 1986.

- [20] A. Burcat, *Combustion Chemistry*, 1st ed., Springer-Verlag, New York, 1984. ([http://www.me.berkeley.edu/gri\\_mech/data/nasa\\_plnm.html](http://www.me.berkeley.edu/gri_mech/data/nasa_plnm.html))
- [21] J. Chang, O. Guralp, Z. Filipi, D. Assanis, T.W. Kuo, P. Najt, R. Rask, *New Heat Transfer Correlation for an HCCI Engine Derived from Measurements of Instantaneous Surface Heat Flux*, SAE Paper No. 2004-01-2996, 2004.
- [22] O. Jahanian, S.A. Jazayeri, *A Comprehensive Study on Natural Gas HCCI Engine Response to Different Initial Conditions via a Thermo-Kinetic Engine Model*, ASME Internal Combustion Engine Division Fall Technical Conference (ICEF2009), Lucerne, Switzerland, 2009.
- [23] O. Jahanian, S.A. Jazayeri, *A Thermo-Kinetic Model Base Study on Natural Gas HCCI Engine Response to Different Initial Conditions*, Int'l Congress on Combustion Engines, Opole, Poland, 2009.
- [24] O. Jahanian, S.A. Jazayeri, *A Single Zone Thermodynamic Model to Investigate the Performance of an HCCI Engine Fueled with Methane*, 12th Annual and 1st International Fluid Dynamic Conference (FD 2009), Babol, Iran, 2009. (in Persian)
- [25] M.P. Halstead, L.J. Krisch, C.P. Quinn, *The Autoignition of Hydrocarbon Fuels at High Temperatures and Pressures*, *Combust. Flame* 30 (1977) 45-60.
- [26] M. Shahbakhti, R. Koch, *Thermo-Kinetic Combustion Modeling of an HCCI Engine to Analyze Ignition Timing for Control Applications*, Spring Technical Meeting Combustion Institute / Canadian Section, 2007.
- [27] K. Swan, M. Shahbakhti, R.C. Koch, *Predicting Start of Combustion Using a Modified Knock Integral method*, SAE Paper No. 2006-01-1086, 2006.
- [28] S.S. Sazhin, E.M. Sazhina, M.R. Heika, C. Marooney, S.V. Mikhalovsky, *The Shell Autoignition Model: A New Mathematical Formulation*, *Combust. Flame* 117 (1999) 529-540.
- [29] H. Hu, J. Keck, *Autoignition of Adiabatically Compressed Combustible Gas Mixtures*, SAE Paper No. 872110, 1987.
- [30] K.R. Nouri, A.F. Mohsenian Rad, *Investigation on the Effects of Using Natural Gas as a Fuel on the Performance of Internal Combustion Engines*, 2nd Conference & Exhibition on CNG & Related Industries, Tehran, Iran, 2009. (in Persian, reproduced from Iranian Fuel Conservation Company (IFCO) reports)
- [31] S. Gordon, B.J. McBride, *Computer Program for Calculation of Complex Chemical Equilibrium Compositions and Applications I. Analysis*, NASA Reference Publication 1311, October 1994.
- [32] A.M. Aceves, D.L. Flowers, C.K. Westbrook, J.R. Smith, R. Dibbe, *A Multi-Zone Model for Prediction of HCCI Combustion and Emissions*, SAE Paper No. 2000-01-0327, 2000.

## Biographies



Omid Jahanian is a PhD graduate from department of mechanical engineering, K. N. Toosi University of Technology. He has carried out his thesis under the supervision of Dr. S. A. Jazayeri. His research interests include simulation analysis of internal combustion engines operating under HCCI mode.



S. Ali Jazayeri is an Associate Professor at department of mechanical engineering, K. N. Toosi University of Technology. His research interests include experimental and simulation analysis of internal combustion engines, hydraulics and fluid mechanics.