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USING GENETIC ALGORITHM and MULTI ZONE COMBUSTION MODEL for OPTIMIZATION of GRI-MECH 3.0 Mechanism in HCCI ENGINES

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ABSTRACT The objective of the present study is to develop a multi-zone combustion model for NG-fueled HCCI engines that could predict engine combustion, performance and emission characteristics. For this purpose, a six-zone combustion model was developed to consider in-homogeneities inside the cylinder, and heat and mass transfer between zones. The natural gas chemistry was described via the GRI-Mech 3.0 mechanism. In most considered operating conditions of this research, hot exhaust gas was blended with fresh fuel/air mixture in the intake manifold. Since GRI-Mech 3.0 mechanism was developed for operating conditions in which there is no EGR gases inside the cylinder charge, and then the mechanism needs to be modified to model the operating conditions with EGR. Therefore, in the current study Arrhenius rate coefficients of the reactions of this mechanism were optimized using genetic algorithm. Finally, the modeling results were compared with experimental data. The results showed the model performance to predict engine various parameters. All engine performance, combustion and emission related parameters showed a good agreement with experimental data.

Keywords HCCI Combustion, NG, Chemical Kinetics, Multi-Zone Model, Genetic Algorithm.

INTRODUCTION

Homogeneous Charge Compression Ignition (HCCI) engines are being considered as a future alternative for diesel engines [Aceves 2000]. In recent years, HCCI engines received many researchers' attention due to its potential to increase thermal efficiency while greatly decreasing NOx and particulate emissions [Noda 2001, Fiveland 2000]. Some disadvantages of HCCI engines are high unburned hydrocarbons (UHC) and heavy carbon monoxide (CO) emissions and low Indicated Mean Effective Pressure (IMEP) [Suzuki 1997, Ishibashi 1996].
Developing a model for HCCI engines is a relatively difficult task; because the model should be able to describe both physical and chemical phenomena inside the combustion chamber. Given that HCCI combustion characteristic is controlled by chemical kinetics [Ogink 2002], considering detailed chemical kinetics in modeling studies seems to be necessary.
Some of recent studies can be summarized as follows:
Aceves et al. [2000] developed a MZCM using KIVA and HCT (Hydrodynamics, Chemistry and Transport). The KIVA code was used to generate temperature and mass distribution during compression stroke up to ignition. Then a 10-zone model was used to simulate the auto-ignition and combustion processes. No heat and mass transfers between zones were allowed.

Ogink and Golovitchev [2002] modeled the complete cycle of a HCCI engine using SENKIN and AVL BOOST software packages. The initial conditions at IVC calculated by AVL BOOST and fed to a MZCM, which used SENKIN. Engine emissions were over- predicted, because, emissions calculated at EVO, but in experimental setup emissions were measured in exhaust port.
Komninos et al. [2004] developed a new MZCM in which heat and mass transfers were taken into account simultaneously but they used global combustion model for HCCI combustion. Later, the authors extended their model and took detailed chemical kinetics into account [2005].
Komninos [2009] investigated the effect of mass transfer on HCCI emission formation using a MZCM. The author concluded the path of HC and CO emission formation in HCCI engines and showed that, mass transfer to crevices volume is the main source of HC and CO formation.
The objective of this study was to construct a MZCM for a NG fueled HCCI engine, which could predict engine combustion, performance and emission parameters simultaneously. For this purpose, a six-zone model was developed and both heat and mass transfers were included in the model. To consider CNG detailed chemical kinetics, GRI-Mech 3.0 mechanism [Smith 2006], which considers 53 species and 325 reactions including NOx chemistry, was employed. GRI-Mech 3.0 chemical kinetic mechanism was developed for natural gas combustion without considering EGR. The main parameters of each chemical mechanism which influence the combustion characteristics (i.e. start of combustion and combustion duration) are the Arrhenius rate coefficients of the reactions. The preliminary modeling results showed that, the mechanism's rate coefficients should be modified to consider the effect of EGR on HCCI combustion. Therefore, the rate coefficients optimization was investigated by a developed genetic algorithm code, which coupled with MZCM.

MODEL DESCRIPTION

As shown in Figure 1, six-zone model includes two core zones, three zones for cylinder wall, cylinder head and piston crown boundary layers, and one zone for crevices volume. Core volume (Vcore) is perfectly centered within the charge, forming an inner cylinder of gas that is surrounded by an outer concentric shell of gas with thickness t1.
To model a physical boundary layer, it is assumed that each zone becomes successively thinner as it approaches cylinder surfaces. Geometric ratio defined by R, which indicates each successive zone is how much thinner than previous zone’s thickness.
Taking crevice regions into account is important for two reasons: they decrease the effective compression ratio and the available chemical energy during high temperature combustion [Komninos 2005]. Both of these reasons lead to a decrease in peak combustion pressure and affect engine performance. Additionally, as a result of low temperature in crevice regions, the charge of these regions doesn’t ignite and because of that, crevices are the main source of HC and CO emissions in HCCI engines. The crevice volume is considered to be constant throughout the engine cycle and estimated to be 3% of the clearance volume [Heywood 1988]. The temperature of crevice regions also assumed to be constant and equal to wall temperature [Heywood 1988, Easley 2001].

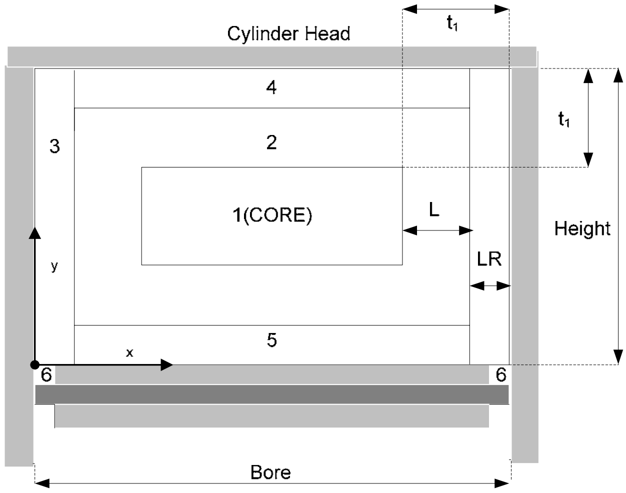

Figure 1. Zone configuration of MZCM

GOVERNING EQUATIONS

In-cylinder mass remains constant, because modeling take place in the closed part of engine cycle. Therefore:

$$\frac{dm_{tot}}{dt} = 0 \qquad (1)$$

m_{tot} : $in-cylinder\ total\ mass\ (kg)$

Mass is transferred between zones to maintain the pressure uniform inside the combustion chamber as follows:

$$\frac{dm_k}{dt} \neq 0 \quad , K = 1, \ldots, N_Z \qquad (2)$$

m_k : mass of k^{th}zone (kg)

N_z : number of zones

The cylinder pressure is calculated at each crank angle (CA) step using the ideal gas relation for all the zones:

$$PV_k = \frac{m_k}{MW_k} R_u T_k , K = 1, \ldots, N_Z \qquad (3)$$

P : $in-cylinder\ \ pressure(Pa)$

V_k : $volume\ \ of\ \ k^{th} zone(m^3)$

MW_k : $molecular\ weight\ of\ k^{th} zone (kg/kmole)$

R_u : $universal\ gas\ constant = 8.314 (J/mol.K)$

T : $temperature\ (K)$

Energy conservation equation and net rate of production equation for each species are also as follows:

$$m_k \overline{c_\upsilon^k} \frac{dT_k}{dt} = -m_k \sum_{i=1}^{N_s} U_i \frac{dY_{i,k}}{dt} - P\frac{dV_k}{dt} + \frac{dQ_k}{dt} \quad (4)$$

$$\frac{dY_{i,k}}{dt} = \frac{\dot{\omega}_{i,k} MW_i}{\rho_k} \quad (5)$$

$\overline{c_v^k}$: $specific\ heat\ for\ k^{th} zone\ (j/kg.K)$

U_i : $Internal\ energy\ of\ the\ i^{th} species\ (j)$

$Y_{i,k}$: $mass\ fraction\ of\ i^{th}\ species\ in\ the\ k^{th} zone$

Q_k : $heat\ transfer\ of\ the\ k^{th} zone\ (j)$

$\dot{\omega}_{i,k}$: $molar\ rate\ of\ production\ of\ i^{th}\ species\ in\ the\ k^{th} zone\ (mole/cm^3.s)$

Convection from in-cylinder mixture to cylinder wall was described using Woschni correlation [Chang 2004].

$$h_c(t) = \beta Height(t)^{-0.2} P(t)^{0.8} T(t)^{-0.73} v(t)^{0.8} \quad (8)$$

β : $correction\ factor\ of\ convectional\ heat\ transfer$

v : $velocity\ (m/s)$

Heat is transferred between zones with a mechanism similar to conduction. Therefore, the heat flux is a function of temperature difference of the neighboring zones and on their mean distance as follows:

$$\dot{q} = -K\frac{dT}{dy} \quad (9)$$

K : $\mathrm{Thermal\ conductivity\ (W/m.K)}$

The total conductivity in equation (9) is calculated based on the approach of Yang and Martin [Yang 1989] and is the sum of a laminar and a turbulent component.

EXPERIMENTAL SETUP AND ENGINE SPECIFICATIONS

Experimental data was obtained from University of Alberta engine research facility and determined using a Waukesha Co-operative fuel research (CFR) single-cylinder engine. The engine was a standard engine with Bore × Stroke (mm) of 82.6 × 114.3 and was modified to operate in HCCI mode at wide open throttle by Hosseini [2007]. Intake mixture temperature was set at constant value. External exhaust was taken right after the exhaust port and re-circulated into the heated intake air (before any fuel injection). A Kistler 6043A water-cooled pressure transducer was used to acquire pressure signal on a 0.1 CAD resolution. Table 1 summarizes the engine specifications for the current experiments.

Table 1
CFR Engine Specifications

Parameter	Specification
Engine Model	Waukesha CFR
Displacement (cc)	612
Throttle	Fully Open
Compression ratio	13.8
Connecting rod length (cm)	24

COMPUTATIONAL PROCEDURE OF MULTI-ZONE COMBUSTION MODEL

Model was developed using FORTRAN programming language. The solver code solves for the unknown variables (mass fraction for each chemical species and temperature for each zone) sequentially (zone by zone) from zone 1 to zone 6, for a user-defined time step. Time step was fixed at 0.1 CA for compression and expansion processes and 0.05 CA for combustion process (40o CA before top dead center (TDC) to 40o after TDC).

The computational procedure of the multi-zone code is completed in two stages. At first, mass of the zones was assumed constant (i.e. the mass transfer among zones was not considered). In order to estimate temperature and composition of the zones, the first law of thermodynamics, simultaneously, with the net rate of production equation for each species was applied.

In the second stage, initially, the cylinder total pressure was calculated. Then, by considering ideal gas law and each zone's defined volume, each zone's new temperature and mass were calculated.

If the computed mass in the second stage differs considerably with considered tolerance of the first stage, in order to equalize pressure, mass transfer among the zones takes place. Because of mass transfer, energy transfer among the zones occurs. Thus, the first law of thermodynamics and the net rate of production step should be calculated again.

GENETIC ALGORITHM

In the current study, genetic algorithm (GA) was applied using a developed FORTRAN90 code. GA code, first recalls GA input parameters from a file, and then it produces a population randomly, within the range +/- 15% around the original rate coefficient values, and by recalling MZCM, it performs an initial estimate of fitness function using this population. After calculating fitness function, GA changes the rate coefficients of mechanism and repeats this procedure again and again, until it attains maximum generation size. At the end, suitable population must be chosen among the answers.
Applied GA calculates fitness function using a weighting method in which weights (w_i) were selected based on functions importance. Fitness function was considered as follows:

$$\text{Fitness Function} = \sum_{i=1}^{n}\left[w_i \times \left| \frac{X_{i,code} - X_{i,test}}{X_{i,test}} \right| \right] \tag{14}$$

The term $\left|\frac{X_{i,code} - X_{i,test}}{X_{i,test}}\right|$, is the ith target function in which, $X_{i,code}$ is the estimated ith variable via MZCM and $X_{i,test}$ is the experimental attained quantity for ith variable. In this work the concerned functions were related to maximum pressure, indicated work of each working cycle and concentration of emissions (e.g. CO, HC and NOx).

RESULTS AND DISCUSSION

This section verifies the introduced MZCM ability of predicting HCCI engine combustion, performance and emission parameters. For this purpose, three different operating conditions were considered which are available in table 2. According to this table equivalence ratio, EGR percentage and fuel mass rate are different for different cases (engine speed and intake temperature are 800 rpm and 413 K for all considered cases).

Table 2 - CFR engine operating conditions for three considered cases

	Case 1	Case 2	Case 3
Equivalence ratio Φ	0.73	0.47	0.31
NG mass rate (mg/s)	107	92.43	82.32
% EGR	41.16	22.15	0
P_{IVC} (bar)	1.56	1.55	1.56

Figure 2, shows the comparison of in-cylinder pressure history between model results and experimental data for three considered cases. As shown in graphs, MZCM adequately captures in-cylinder pressure during the compression, combustion and expansion periods for all of the selected operating conditions, and model has a good performance over a wide range of operating conditions. Figure 2, also illustrates the original GRI-Mech 3.0 mechanism results. It is evident that, original combustion parameters lead to a significant disagreement between model and experimental results. Therefore, the Arrhenius rate coefficients of reactions need to be optimized. For case 3, where there is no EGR, the original GRI-mech 3.0 mechanism has better results than other three cases.

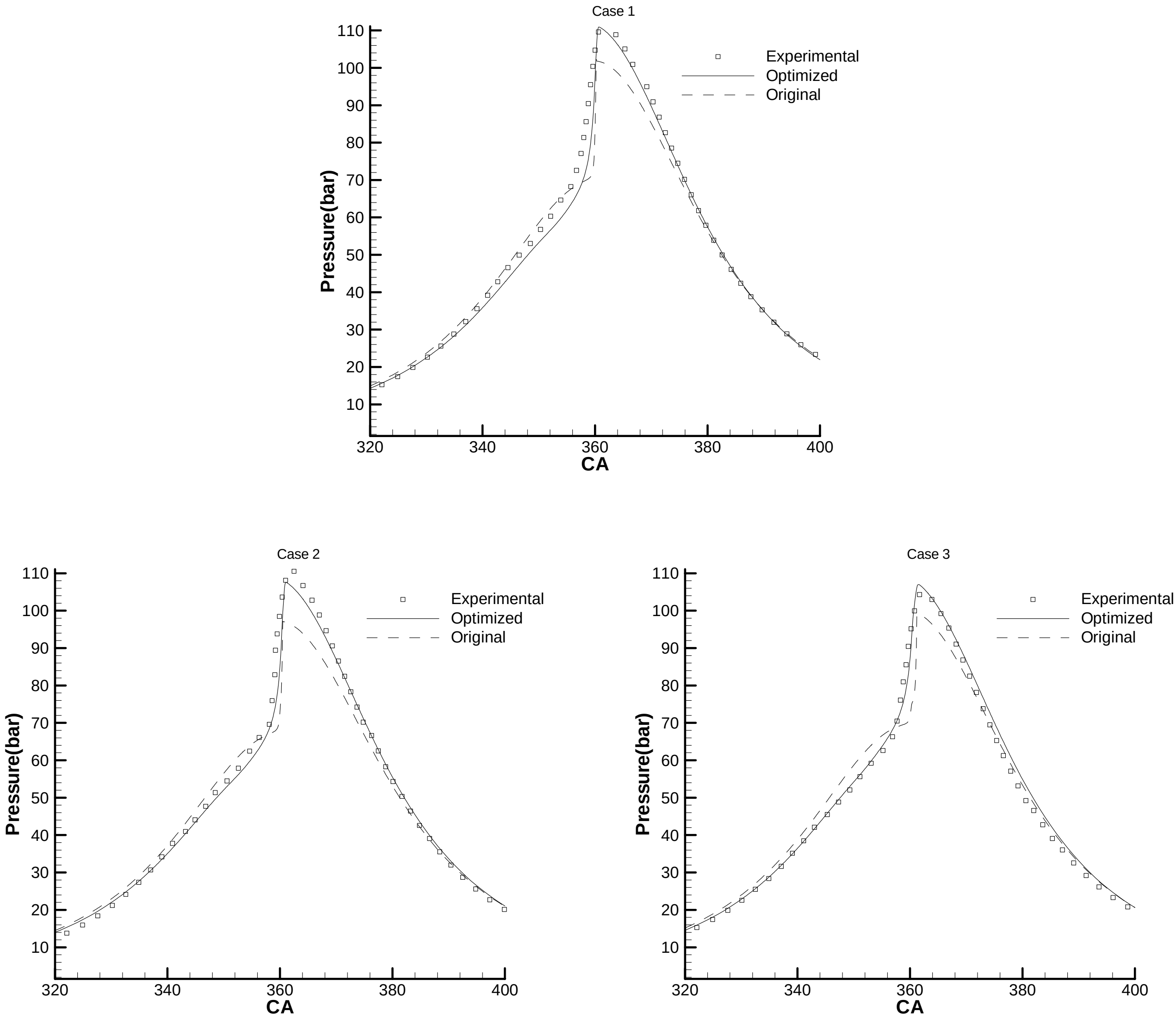

Figure 2. In-cylinder pressure history for three considered cases

Table 3, compares predicted NOx, UHC and CO emissions via MZCM at EVO, with experimental data, for all cases. This table shows that MZCM could predict HC and CO emissions with acceptable accuracy. Additionally, NOx emissions are not a concern in HCCI combustion, since they remain at a very low level.

Table 3 – Comparison of measured and calculated emissions

	Case 1		Case 2		Case 3	
Species	calculated	measured	calculated	measured	calculated	measured
NOx(ppm)	8.63	13.22	5.87	8.32	1.67	0.39
UHC(ppm)	4907.76	4646.85	3998.35	4265.06	3822.1	3918.99
CO (%)	0.083	0.07	0.085	0.06	0.068	0.07

As discussed above, the MZCM simulates pressure traces accurately over a wide range of different operating condition. Beyond matching pressure traces, the engine parameters calculated from the model results were compared with the experimental average engine parameters (Figure 3). The interesting parameters are indicated mean effective pressure (IMEP), start of combustion timing (SOC), combustion duration (CD), and thermal efficiency. SOC and CD are the key measures of combustion behavior, while IMEP and thermal efficiency stand for engine performance. The definition of SOC adopted here was the point of maximum pressure rise rate and the CD was defined as the interval from 10% to 90% of pressure rise due to main combustion [Huang 2001].
According to Figure 3, start of combustion, which strongly depends on chemical kinetics in HCCI engines, was predicted accurately. Combustion duration, which depends on mixture temperature, in-homogeneity and properties, was under predicted in all cases; the reason is that, it is difficult to measure CD of high octane number fuels. Therefore, experimental combustion durations are greater than predicted ones. Since pressure traces were predicted almost accurately, IMEP and thermal efficiency were predicted well.

CONCLUSION

An HCCI, NG fueled engine was modeled using a multi-zone combustion model. The GRI-Mech 3.0 mechanism was used to consider detail chemical kinetics. In order to improve model results for different operating conditions, when EGR was applied, GRI-Mech 3.0 mechanism’s rate coefficients should be optimized. Three different operating conditions were selected to evaluate and validate model efficiency. Comparison of model and experimental results showed that, model could predict combustion, emission and performance characteristic with an acceptable accuracy.
The following conclusions have been drawn:

1. Considering both heat and mass transfer with detailed chemical kinetics in multi-zone combustion models, lead to a good emission and performance prediction.
2. The GA might be used in the hydrocarbons chemical kinetic mechanism development by the reactions rate coefficients adjustment.
3. Fitness function, based on maximum pressure, indicated work and emission concentration might be employed, as an effective parameter, in the proposed mechanism improvement in order to forecast combustion and performance parameters by MZCM.

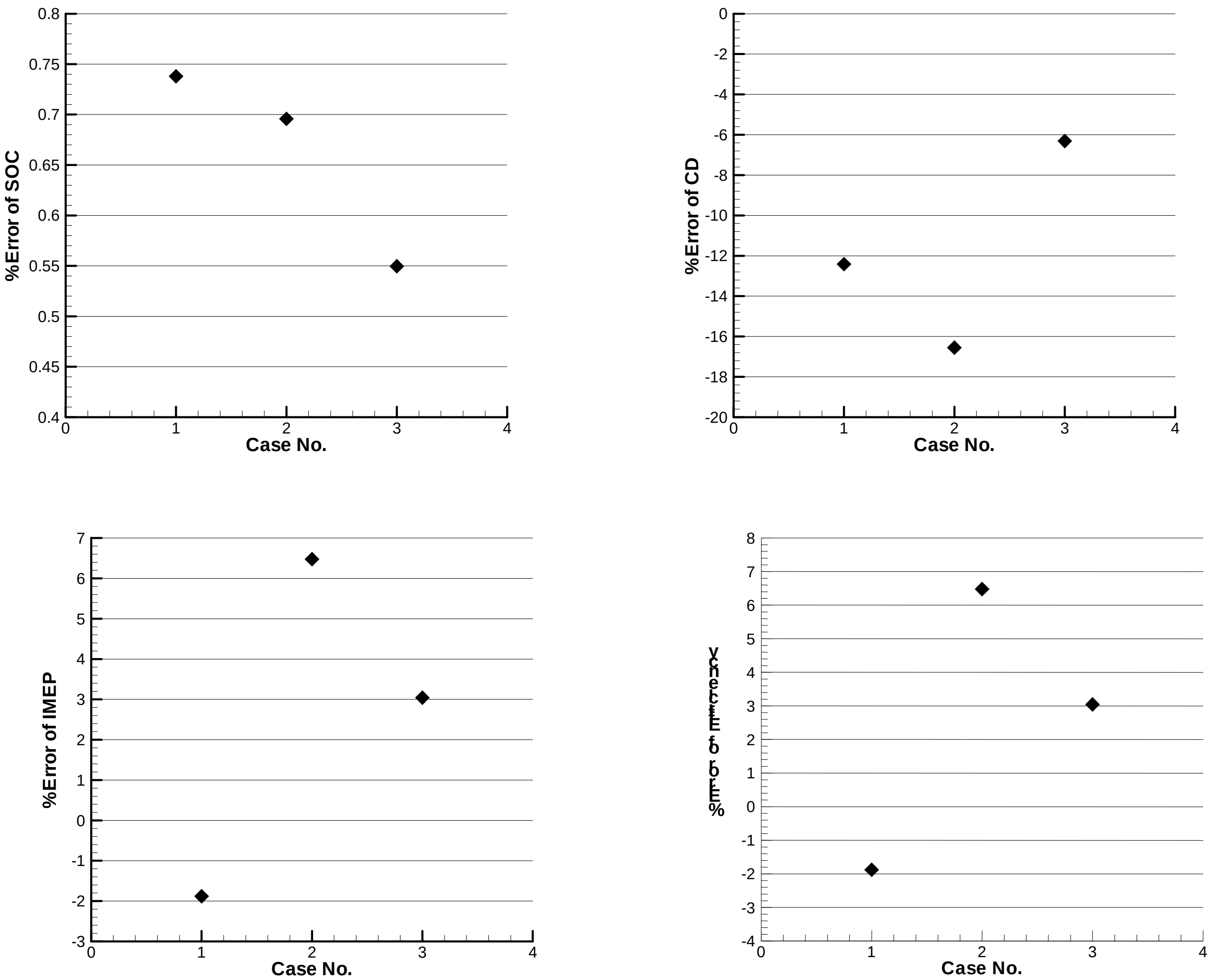

Figure 3. Performance of MZCM on some engine parameters of the HCCI engine

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