

## INVESTIGATION ON EFFECT OF EQUIVALENCE RATIO AND ENGINE SPEED ON HOMOGENEOUS CHARGE COMPRESSION IGNITION COMBUSTION USING CHEMISTRY BASED CFD CODE

by

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*Combustion in a large-bore natural gas fuelled diesel engine operating under homogeneous charge compression ignition mode at various operating conditions is investigated in the present paper. Computational fluid dynamics model with integrated chemistry solver is utilized and methane is used as surrogate of natural gas fuel. Detailed chemical kinetics mechanism is used for simulation of methane combustion. The model results are validated using experimental data by Aceves, et al., conducted on the single cylinder Volvo TD100 engine operating at homogeneous charge compression ignition conditions. After verification of model predictions using in-cylinder pressure histories, the effect of varying equivalence ratio and engine speed on combustion parameters of the engine is studied. Results indicate that increasing engine speed provides shorter time for combustion at the same equivalence ratio such that at higher engine speeds, with constant equivalence ratio, combustion misfires. At lower engine speed, ignition delay is shortened and combustion advances. It was observed that increasing the equivalence ratio retards the combustion due to compressive heating effect in one of the test cases at lower initial pressure. Peak pressure magnitude is increased at higher equivalence ratios due to higher energy input.*

Key words: *computational fluid dynamics, chemistry, equivalence ratio, homogeneous charge compression ignition, engine speed*

### Introduction

Nowadays, with the crisis of depletion of energy resources and environmental pollution, a lot of researches are being done to improve thermal efficiency and to control and reduce emission trade-off on internal combustion engines. Recently, an alternative combustion technology known as homogeneous charge compression ignition (HCCI) has emerged with a potential to achieve high efficiencies and dramatic reduction of nitrogen oxide and particulate emissions [1-4].

Major concerns related to HCCI combustion are control of the combustion phasing under a wide range of engine operating conditions or high unburned hydrocarbon and carbon monoxide emissions due to the incomplete combustion [5, 6]. In the recent decades, development of more comprehensive flow field models has allowed study of different combustion parameters at

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every desired point and time within the combustion chamber for conventional diesel and spark ignition and also newer engines such as HCCI. Commercial codes such as AVL fire has been used to model combustion and emission formation in complex chamber geometries, as in indirect injection diesel engines [7]. Various numerical models have been developed to investigate the HCCI concept such as the single-zone and multi-zone models.

Multi-dimensional computational fluid dynamics (CFD) modeling with detailed chemistry can provide the most accurate predictions which would also require great computing power. Integrated detailed chemical kinetics and KIVA code [8] was used to study the combustion phasing characteristics in an HCCI engine. Results showed that proper combustion phasing can be captured by accounting for effects of turbulence on reaction rates. In another attempt, coupled CFD/chemistry was used to study the cool flame effect on HCCI combustion of n-butane and PRF 70 fuels [9]. Results showed that cool flame energy release alters the thermodynamic state of the mixture which can significantly affect the subsequent hot ignition. Engine speed and cyclic dispersion was investigated experimentally [10]. Their results show that the duration of low temperature reaction is of fundamental importance in HCCI combustion at higher engine speeds. At higher engine speeds, low temperature reaction duration and negative temperature coefficient increase. Machrafi and Cavadiasa [11] studied on effect of inlet temperature, the equivalence ratio and the compression ratio on the combustion of n-heptane and primary reference fuels in an HCCI engine using experiments and simulation methods. They showed that increasing inlet temperature reduces ignition delay due to higher energy input. However, they concluded that higher equivalence ratio does not necessarily mean shorter ignition delay which is due to compressive heating effect that reduces gas temperature at compression.

Kobayashi *et al.* [12] investigated the possibility of a turbocharged natural gas fueled HCCI engine experimentally. They showed that the HCCI engine has a great potential to increase the power generating efficiency of combined heat and power (CHP) at small scales with considerably low values of  $\text{NO}_x$  emission. Nobakht *et al.* [13] developed a 6 zoned multi-zone combustion model to investigate parameters affecting natural gas combustion in an HCCI engine. Results showed that the equivalence ratio and inlet pressure were the most effective parameters on the combustion phasing and performance of the engine. Zhang *et al.* [14] studied the premixed flame speed in a dimethyl ether fueled HCCI engine. They concluded that the flame speed tends to increase with the increase of crank angle and the increment rate is higher at cool flame. It was demonstrated that initial temperature and pressure do not have a considerable effect on the magnitude of flame speed.

In the present paper, a CFD model is used with integrated chemistry solver, to simulate the combustion process in a natural gas fuelled Volvo TD100 diesel engine operating under HCCI engine conditions. Model predictions are validated using experimental measurements [6]. The effect of equivalence ratio and engine speed on combustion related parameters is investigated.

### The computational model

HCCI combustion is highly dependent on fuel oxidation chemistry. In order to simulate this, optimizing of integrated chemical kinetics mechanisms and flow simulations is essential. The KIVA-3V code [15] was selected as 3D-CFD framework for simulations of reactive fluid flow. KIVA uses finite-volume, temporal-differencing scheme in solution procedures of three dimensional conservation equations and turbulence at the same time. This solution procedure, namely the arbitrary Lagrangian-Eulerian (ALE) method, decouples calculations of the

diffusion and convection terms from chemical source terms. Hence, each computational cell can be treated as a homogeneously mixed reactor at each time-step. Continuity equation for species  $m$  and energy equation in terms of specific internal energy are formulated in KIVA as given in eqs. (1) and (2) [16]:

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

$$\frac{\partial(\rho I)}{\partial t} + \nabla(\rho u I) = -P \nabla u - (1 - A_0) \sigma : \nabla u - \nabla J + A_0 \rho \varepsilon + \dot{Q}^c + \dot{Q}^s \quad (2)$$

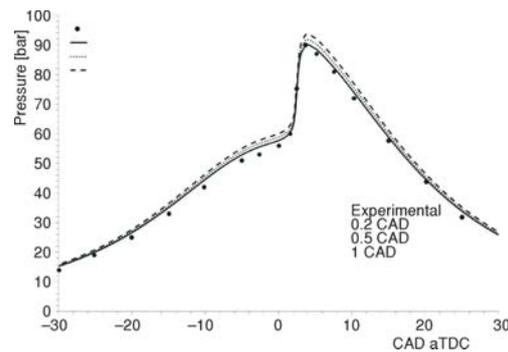
In the equations,  $\dot{\rho}_m^c$  is the density rate of change of species  $m$ , and  $\dot{Q}^c$  are the source terms to be calculated by combustion model as eqs. (3) and (4) [9]:

$$\dot{\rho}_m^c = W_m \dot{\omega}_m \quad (3)$$

$$\dot{Q}^c = - \sum_{m=1}^M \dot{\omega}_m (\Delta h_f^\circ)_m \quad (4)$$

To calculate the molar production rate of chemical species participated in chemical kinetics mechanism, the gas phase kinetics library of CHEMKIN-II [15] is integrated into KIVA code. In this procedure, the KIVA chemistry subroutine has been replaced by a new subroutine developed to perform chemistry solutions. For methane combustion simulation, the DRM 22 mechanism of Berkley University [17], reduced from GRI-MECH mechanism which is including 26 species and 107 reactions is used. Closed cycle simulations start from inlet valve closure (IVC) and end at exhaust valve opening (EVO). A preliminary study showed that a time step value of 0.2 CAD (crank angle degree) degree was small enough to provide good predictions while keeping the computational time reasonable. Results for the mean pressure vs. CAD at different time steps can be seen in fig. 1. It can be seen that a time step of 1 CAD tends to overestimate the pressure magnitudes.

Heat transfer subroutine is also modified in the current model to calculate wall heat flux based on Han and Reitz [18] formulation and The RNG  $k-\varepsilon$  model is used as turbulence model. The numerical model for Volvo TD100 engine with geometrical specifications on tab. 1 is generated by ANSYS ICEM CFD software. Considering the symmetry of the model and the computational heavy nature of the coupled



**Figure 1. Comparison of predicted and experimental pressure histories at constant 1000 rpm engine speed with no pressure boost**

**Table 1. Experimental engine specifications [6]**

Bore × stroke	120.65 mm × 140 mm
Connecting rod length	260 mm
Engine speed	1000 rpm
Trapped compression ratio	19:1
Geometrical compression ratio	21:1
IVC	-167 CAD aTDC
EVO	140 CAD aTDC
Displacement volume	1600 cm <sup>3</sup>
Fuel	Natural gas

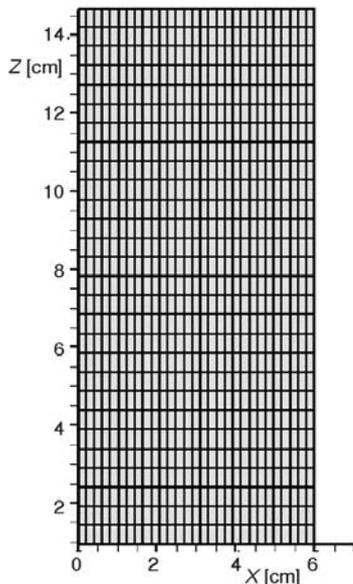


Figure 2. 2-D numerical grid at IVC

model, the problem was solved for a 2-D section of the whole geometry with periodic boundary conditions. Figure 2 shows the numerical grid which contains approximately 1000 cells at IVC.

### Results and discussion

The simulations are verified using experimental data [6]. The operating conditions for cases under study are listed in tab. 2. Test cases are obtained by increasing the initial boost pressure from the base case (0 bar boost) up to 2 bars. All cases are running at 1000 rpm engine speed at constant trapped compression ratio of 19:1. The wall temperatures for cylinder wall, head and piston surface are considered con-

Table 2. Operating conditions [4]

Case study	0 bar pressure boost	1 bar pressure boost	2 bar pressure boost
Intake temperature, [K]	424	352	323
Equivalence ratio	0.379	0.292	0.259

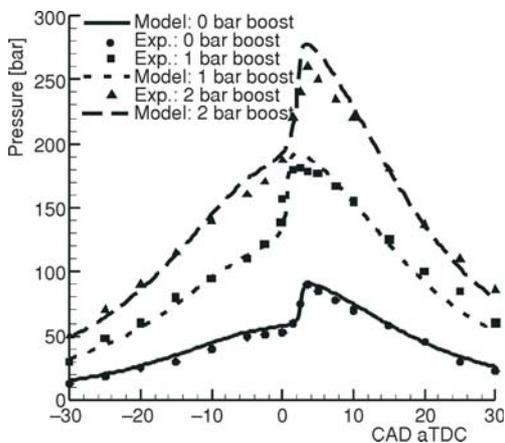
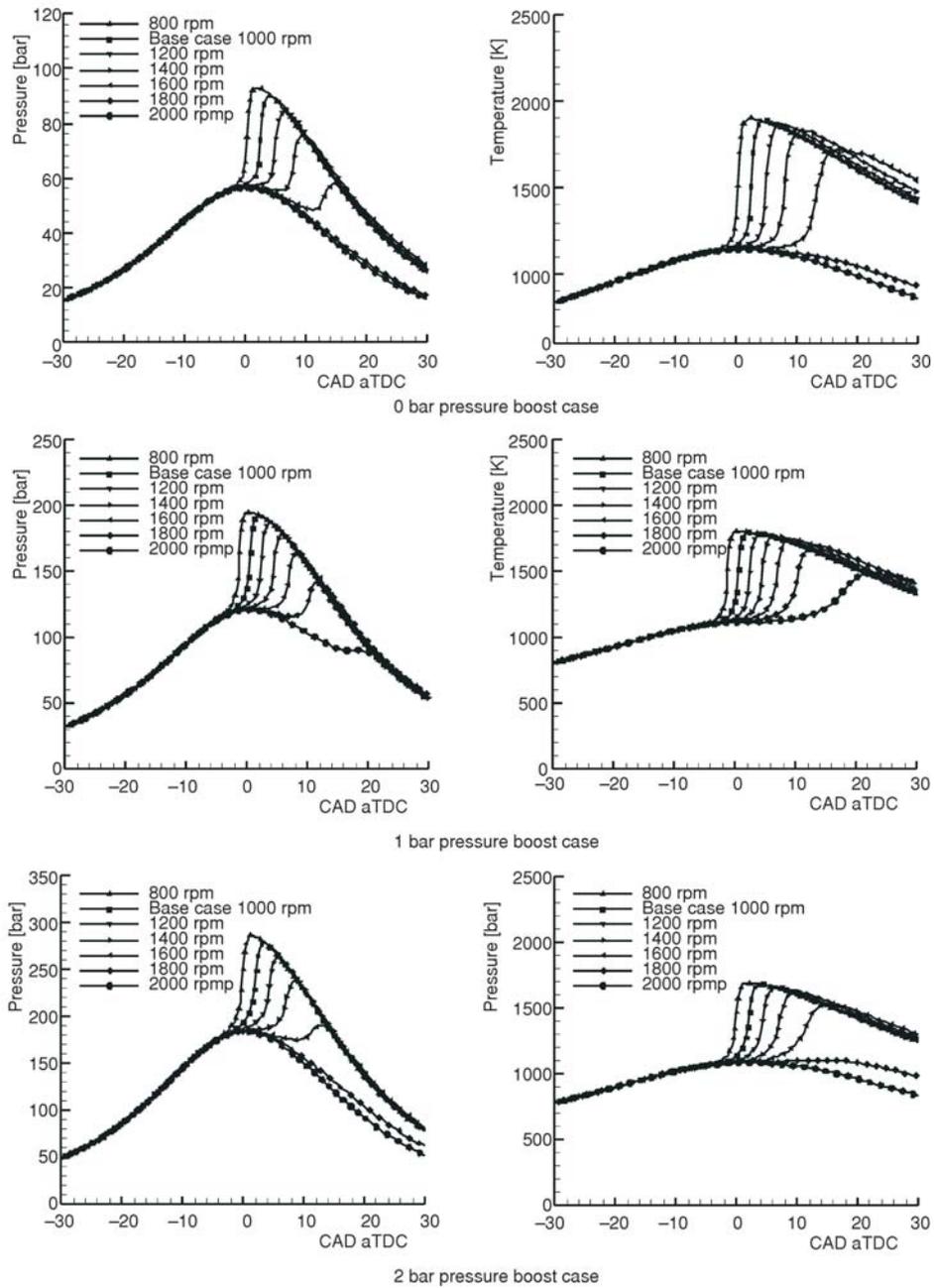


Figure 3. Comparison of predicted and experimental pressure histories at constant 1000 rpm speed

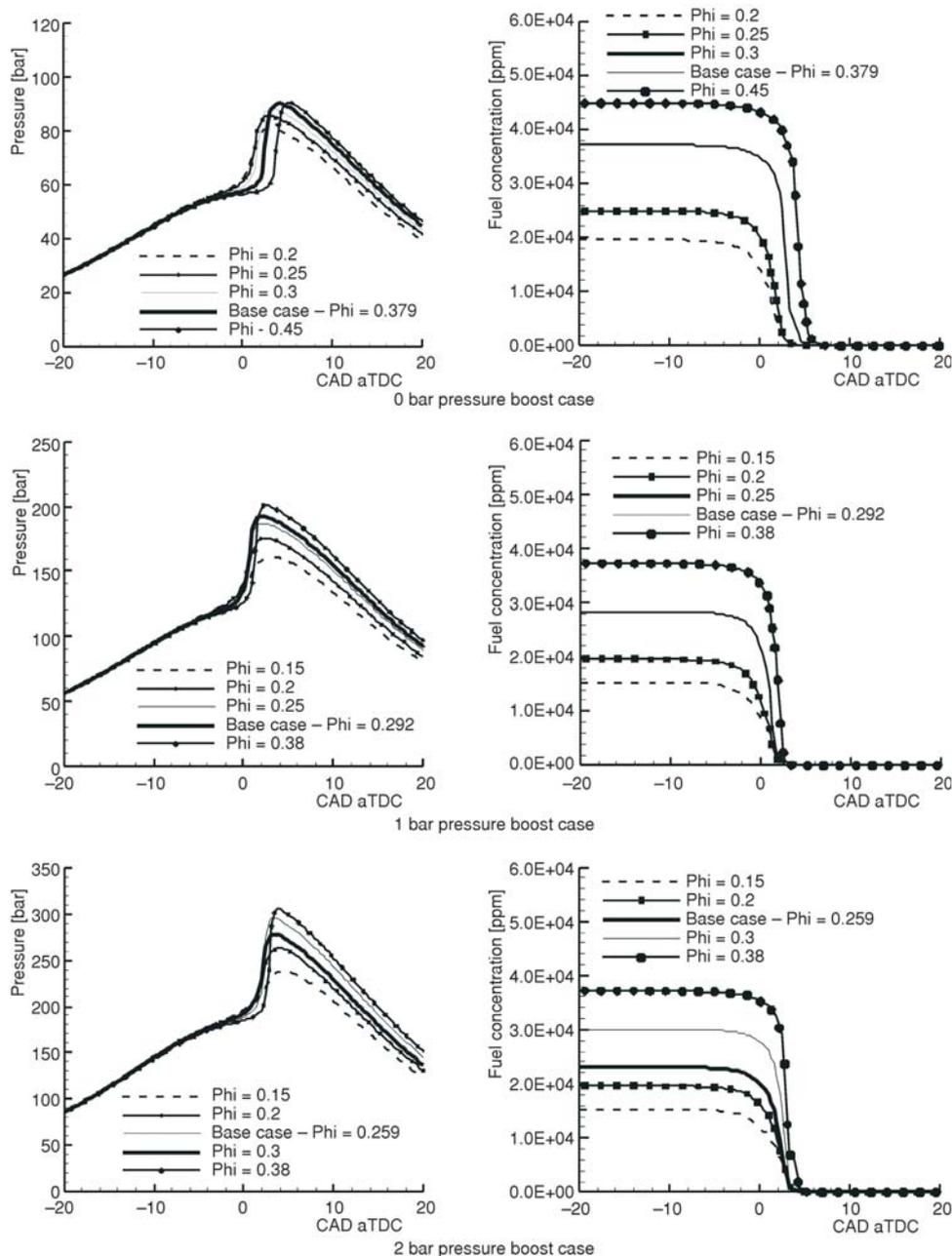
stant as 422 K, 478 K, and 437 K respectively [6]. Figure 3 shows the comparison between measured [6] and predicted data for the three base cases on tab. 2. It can be seen that the model predictions for mean in-cylinder pressure traces, peak pressure magnitude and location agree well with experiments, especially at lower boost pressure test cases. The results are comparable with the findings of Aceves *et al.* [6] using multi-zone model with detailed reaction mechanism including 1125 elementary reactions compared to current model's 107 reaction scheme. This good agreement between the measured and model computed results for the engine operating conditions gives confidence in the model predictions, and suggests that the model may be used to explore concepts about effects of equivalence ratio on combustion process at various engine speeds.

Figure 4 shows the results for mean in-cylinder pressure and temperature histories for different cases at various engine speeds. It can be concluded that considering constant equivalence ratio, combustion phasing is delayed and ultimately misfiring occurs at high engine speeds (*i. e.* 1800 and 2000 rpm for 0 bar pressure boost case) whereas, at lower engine speeds, ignition delay is shortened. Increasing the engine speed also corresponds with lower peak pressure and temperature magnitude which is more pronounced at 0 and 2 bar pressure boost cases.



**Figure 4.** Mean in-cylinder pressure and temperature histories for different cases at various engine speeds

Figure 5 depicts the effect of equivalence ratio on combustion of methane at three test cases. For this purpose, pressure and fuel concentration histories are presented. As methane is a



**Figure 5.** Pressure traces and fuel concentrations for different cases at various equivalence ratios (*i. e.*  $\Phi$ )

high octane fuel, it has a higher resistance in overcoming the compressive heating effect [11]. This is evident from the figures as it can be seen that increasing the equivalence ratio, while keeping the initial mixture temperature constant, tends to increase the ignition delay and de-

creasing fuel-air ratio results in advancing the ignition. This is more pronounced in 0 bar boost pressure case due to its lower initial pressure compared to 1 and 2 bar boost pressure cases. It can also be said that initial mixture temperature does not have influential effect on the compromise between compressive heating and energy input. However, it can be said that at higher equivalence ratios, peak pressure magnitude increases due to higher energy input. Burn rate also seems to be increased at delayed combustion as methane concentrations is depleted rapidly.

Figure 6 shows the contours of methane concentration at various selected crank angles during combustion phase for equivalence ratio of 0.2 for test cases. Combustion starts from hot ignition spots in the center of the chamber where temperature is higher and then proceeds to the whole chamber. Considering the results indicated on fig. 4 and the contours in this figure, the ignition delay and faster combustion rate is evident at higher boost pressure cases. At 0 bar boost case, burn rate is slower compared to 1 and 2 bar boost cases and combustion starts at approximately  $-5$  CAD aTDC and majority of fuel is consumed after top dead center. Whereas in 2 bar boost case, there is no evidence of combustion at 1 CAD aTDC, after which, the fuel burns rapidly over the next 2 CAD.

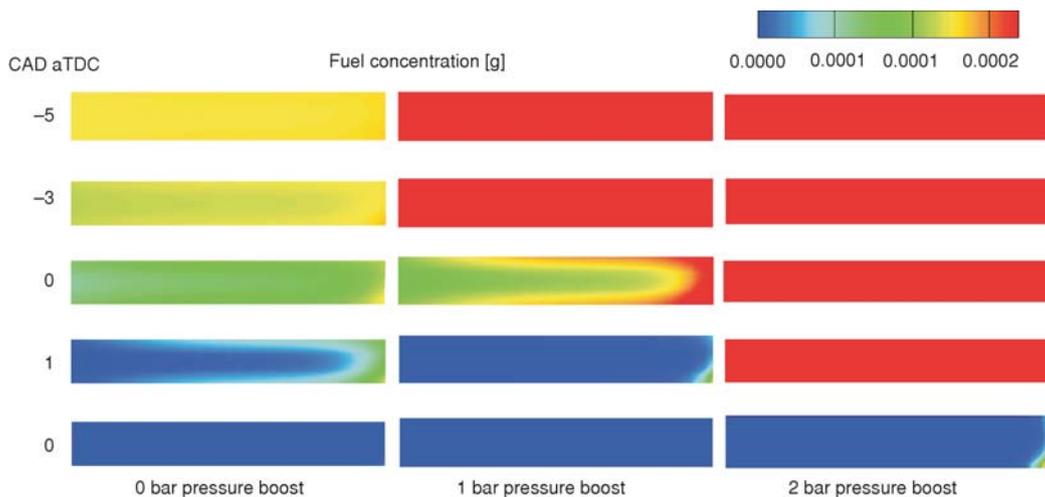


Figure 6. Combustion of methane at  $\Phi = 0.2$  for test cases

## Conclusions

This paper was dedicated to study the effect of equivalence ratio and engine speed on the combustion process in an HCCI engine using KIVA 3-V code with integrated chemistry, and the following results were obtained.

- It was seen that the results of current model agrees well with experiments and that this model is capable of comparable predictions with a ten times reduced chemical kinetic mechanism.
- Results indicated that at higher engine speeds, with constant equivalence ratio, combustion tends to misfire, whereas, at lower speed, ignition delay is shortened.
- Increasing the engine speed also corresponds with lower peak pressure and temperature magnitude which is more pronounced at 0 and 2 bar pressure boost cases.
- It was observed that increasing the equivalence ratio retards the combustion due to compressive heating in 0 bar boost case but does not have considerable effect on ignition delay in 1 and 2 bar boost cases.

- Overall, peak pressure magnitude is increased at higher equivalence ratio due to higher energy input.
- Methane burn rate is slower at increased boost pressure cases while the combustion is retarded.

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### References

- [1] Atkins, M. J., Koch, C. R., The Effect of Fuel Octane and Diluent on Homogeneous Charge Compression Ignition Combustion, *Proc. Inst. Mech. Eng. Part D, Journal of Automobile Engineering*, 219 (2005), 5, pp. 665-675
- [2] Xingcai, L., *et al.*, Experimental Study on the Cycle-by-Cycle Variations of Homogeneous Charge Compression Ignition Combustion Using Primary Reference Fuels and Their Mixtures, *Proc. Inst. Mech. Eng. D-J AUT* (2007); DOI: 10.1243/09544070JAUTO481
- [3] Saxena, S., Bedoya, I. D., Fundamental Phenomena Affecting Low Temperature Combustion and HCCI Engines, High Load Limits, and Strategies for Extending these Limits, *Prog. Energ. Combust.*, 39 (2013), 5, pp. 457-488
- [4] Yao, M., *et al.*, Progress and Recent Trends in Homogeneous Charge Compression Ignition (HCCI) Engines, *Prog. Energ. Combust.*, 35 (2009), 5, pp. 398-497
- [5] Maroteaux, F., Noel, L., Development of a Reduced n-Heptane Oxidation Mechanism for HCCI Combustion Modelling, *Combust. Flame*, 146 (2006), 1-2, pp. 246
- [6] Aceves, S. M., *et al.*, A Multi-Zone Model for Prediction of HCCI Combustion and Emissions, SAE technical paper 2000-01-0327, 2000
- [7] Barzegar, R., *et al.*, CFD Simulation of the Combustion Process, Emission Formation and the Flow Field in an In-Direct Injection Diesel Engine, *Thermal Science*, 17 (2013), 1, pp. 11-23
- [8] Kong, S. C., *et al.*, Modelling and Experiments of HCCI Engine Combustion Using Detailed Chemical Kinetics with Multi-Dimensional CFD, SAE technical paper 2001-01-1026, 2001
- [9] Sohm, V., *et al.*, A Computational Investigation into the Cool Flame Region in HCCI Combustion, SAE technical paper 2004-01-0552, 2004
- [10] Ebrahimi, R., Desmet, B., An Experimental Investigation on Engine Speed and Cyclic Dispersion in an HCCI Engine, *Fuel*, 88 (2010)8, pp. 2149-2156
- [11] Machrafi, H., Cavadiasa, S., An Experimental and Numerical Analysis of the Influence of the Inlet Temperature, Equivalence Ratio and Compression Ratio on the HCCI Auto-Ignition Process of Primary Reference Fuels in an Engine, *Fuel Processing Technology*, 89 (2008), 11, pp. 1218-1226
- [12] Kobayashi, K., *et al.*, Development of HCCI Natural Gas Engines, *Journal of Natural Gas Science and Engineering*, 3 (2011), 5, pp. 651-656
- [13] Nobakht, A., *et al.*, A Parametric Study on Natural Gas Fueled HCCI Combustion Engine Using a Multi-Zone Combustion Model, *Fuel*, 90 (2011), 4, pp. 1508-1514
- [14] Zhang, M., *et al.*, Numerical Study of Effects of the Intermediates and Initial Conditions on Flame Propagation in a Real HCCI Engine, *Thermal Science*, 18 (2014), 1, pp. 79-87
- [15] Amsden, A., KIVA-3V: A Block-Structured KIVA Program for Engines with Vertical or Canted Valves. LA-13313-MS, 1997
- [16] Kee, R. J., *et al.*, CHEMKIN-II: A FORTRAN Chemical Kinetics Package for the Analyses of Gas Phase Chemical Kinetics. Sandia Report (1989); SAND 89-8009
- [17] \*\*\*, <http://www.me.berkeley.edu/DRM/>
- [18] Han, Z., Reitz, R. D., A Temperature Wall Function Formulation for Variable-Density Turbulent Flows with Application to Engine Convective Heat Transfer Modelling, *Int. J. Heat Mass Transfer*, 40 (1997), 3, pp. 613-625

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