NUMERICAL STUDY OF EFFECTS OF THE INTERMEDIATES AND INITIAL CONDITIONS ON FLAME PROPAGATION IN A REAL HOMOGENEOUS CHARGE COMPRESSION IGNITION ENGINE

by

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The premixed flame speed under a small four stock homogeneous charge compression ignition engine fueled with dimethyl ether was investigated. The effects of intermediate species, initial temperature, initial pressure, exhaust gas re-circulation, and equivalence ratio were studied compared to the baseline condition. Results show that under all conditions, the flame speeds calculated without intermediates are larger than those considered the intermediates. Flame speeds increase with the increase of crank angle. The increasing rate is divided into three regions and the increasing rate is obviously large when low temperature heat release occurs. Initial temperature and pressure only affect the crank angle of flame speed, but have little influence on its value. Equivalence ratio and exhaust gas re-circulation ratio not only distinctly decrease the flame speed but also advance the crank angle of flame speed.

Key words: *homogeneous charge compression ignition engine, dimethyl ether, flame propagation, intermediate species*

Introduction

With increasing concern on the depletion of fossil fuel and environmental protection, the research and development of high performance internal combustion engines have been attracting more attention in the past decades. The homogeneous charge compression ignition (HCCI) engine, combining the advantages of both spark-ignition (SI) engine and compression-ignition (CI) engine, is a promising approach to achieve high-efficiency and low-emissions simultaneously [1-5]. However, there still remain many problems when it was applied to a production engine. The difficulties of HCCI engine have mainly two aspects. Firstly, the auto-ignition timing of HCCI, which is controlled by the chemical kinetics of the mixtures, is much complicated comparing to the conventional SI and CI engines, whose combustion timing are controlled by the spark timing and injection timing, respectively. Secondly, the operating range of HCCI is narrow and cannot meet the wide operating requirement of real engine. The low load suffers from low combustion efficiency and high HC, CO emissions due to the bulk gas incomplete combustion and low oxidation of formed HC and CO and the possible misfire. The high load is limited by the knocking due to the simultaneous ignition of the mixtures which leads to extremely high pressure rise rate (PPR) and pressure.

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To solve the above two problems, many potential control methods have been tested for the extension of the operating range. Those two approaches are mainly focused the gasoline like (single-ignition) HCCI and diesel like (two-ignition) HCCI. Mixture and/or thermal stratification has been introduced by various methods such as the direct injection (DI) [6] and pilot injection [7-9] to prevent all the mixtures in the cylinder from being ignited simultaneously. Exhaust gas re-circulation (EGR) [10-14], various fuels [15-17], and fuel blends [18, 19] were used to adjust the heat release history. However, the operating range is still limited to a relatively lower load. When HCCI engine operates at high load, knocking phenomena will occur due to the simultaneous ignition of the whole mixtures in the cylinder, leading to a high pressure rise. However, in a real engine, there always exists some inhomogeneity of fuel/air mixture and temperature in the cylinder caused by the mixing, EGR, heat transfer and the way that the fuel and air introduced. Since the absolute homogenous condition is hard to realize, usually some positions are firstly auto-ignited and the rest mixtures are consumed by flame propagation or compression auto-ignition. This phenomenon is due to the stratification or the degree of inhomogeneous regionally in the real HCCI engine. Researches of the degree of inhomogeneous have been made numerically and experimentally [10, 12, 20]. The results showed that stratification (mixture and/or thermal stratification) could improve the performance of the HCCI engine by decreasing PPR and extend the operating range to a relatively high load. This indicated that if there exists a portion of the mixtures that were ignited by flame propagation instead of simultaneous ignition of all the mixtures, PRR could be reduced and operating range could be extended. This kind of HCCI engine works between the spark ignition engine where all mixtures are ignited by flame propagation, and the compression ignition engine where there is no flame propagation in the cylinder [2, 21]. The effects of initial conditions on flame propagation are very important to the understanding of the relationship between combustion through flame propagation and through compression auto-ignition as illustrated in fig. 1. It was supposed that if a higher flame speed is presented during the compression stroke, a larger portion of the mixtures would be ignited by flame propagation, resulting in the decrease of PPR and extension of operating range. The intermediates play very important role in the combustion, especially during the compression stroke between the timing of low temperature heat release (LTHR) start and the timing of high temperature heat release(HTHR) start. Since only a small fraction of heat release is released so the temperature is low during this range. The objective of this paper is to study the effects of intermediates and initial conditions on the flame propagation of a real HCCI engine. This study will help the understanding of the relationship between the ignition/combustion by flame propagation and ignition/combustion by compression auto-ignition. Flame propagation speed under various crank angles between LTHR and HTHR were calculated. The effects of initial temperature, initial pressure, equivalence ratio, EGR ratio and intermediates on flame propagation were analyzed.

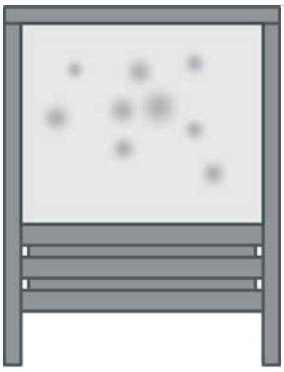

Figure 1. Schematic of compression auto-ignition and flame propagation in a real HCCI engine

Calculation method and procedures

Fuel selection and the HCCI engine

Dimethyl ether (DME) was used in the study even though HCCI engine can be operated by using a variety of fuels [15, 16, 18, 22], such as primary reference fuels (PRF) [15, 22, 23]. DME is regarded as a promising clean fuel for engines for its two stage heat release. DME was operated on HCCI engine by many researchers [22, 24-26]. Two stage ignition is LTHR or cool-flame chemistry [12, 26] and HTHR. Total heat release of HTHR is about 3 to 9 times larger than that of LTHR. The heat release of LTHR is the initial oxidation of fuel and the preparation of the bulk cylinder combustion. Properties of DME are given in tab. 1. A small four-stroke engine is used for the calculation, and engine parameters are given in tab. 2.

Table 1. Properties of DME

Fuel	DME
Chem. formula	CH_3OCH_3
Comp. (C/H/O) [mass %]	52.2/34.8/12
Molar mass [gmol^{-1}]	46.07
Lower heating value [MJkg^{-1}]	28.8
Stoichiometric air/fuel ratio	14.29
Heat release in LTHR	10~30%
Heat release in HTHR	70~90%

Table 2. Parameters of the modeled HCCI engine

Bore × stroke [mm]	112 × 115
Compression ratio	9.6
Displacement [mm^3]	1132
Engine speed (rpm)	1500
Intake valve open (aTDC)	–132
Exhaust valve close (aTDC)	132

The calculation method

HCCI engine and flame speed under various crank angles were calculated by using SENKIN [27] and PREMIX [28] of CHEMKIN-PRO [29] with Curran's DME mechanism [30]. The Curran's DME mechanism consists of 78 chemical species and 336 chemical reactions which has been validated by jet-stirred reactor data at pressure up to 1.0 MPa and ignition delay times at pressure up to 4.0 MPa. Calculation is carried out based on the following assumptions: (1) A premixed mixture is homogeneous. (2) Total mass is preserved before and after reactions. (3) No heat transfer. (4) Ideal gas. Upwind differencing on the convective term was used to solve the energy equation and the mixtures averaged model was used for transport properties calculation. A HCCI engine under specific initial temperature and pressure condition was calculated by using the adiabatic HCCI model of SENKIN. Heat release rate (HRR), temperature and pressure histories versus crank angle are obtained and used as the conditions for flame speed calculation. Calculation is carried out between the crank angles of LTHR starting and HTHR starting. The definition of LTHR and HTHR starting are shown in fig. 2. The LTHR starting is the timing where HRR reaches 1.0 J/CA and the HTHR starting is the timing where the mole fraction of H_2O_2 reaches its maximum value [31].

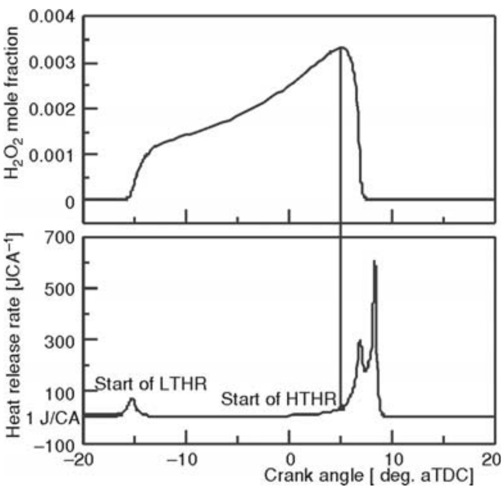

Figure 2. Definition of the LTHR and HTHR start crank angle

The convergence of flame speed calculation is controlled by the two criteria, CURV and GRAD [28]. CURV and GRAD are adaptive mesh parameters, which control the number of grid, points inserted in regions of high curvature and high gradient, respectively. Smaller values of CURV and GRAD cause more grid points to be used. The effect of CURV and GRAD on

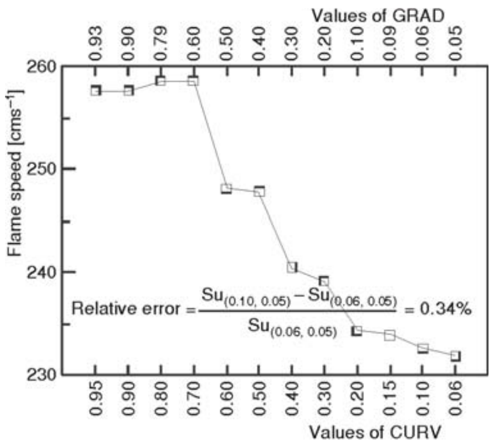

Figure 3. Effect of CURV and GRAD on flame speed calculation

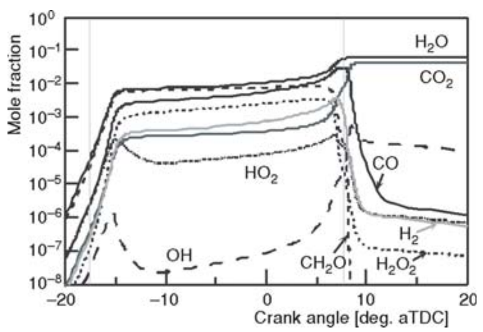

Figure 4. Intermediate species considered in the flame speed calculation

flame speed calculation is given in fig. 3. Flame speed keeps almost constantly when CURV is 0.20 and GRAD = 0.10, the relative error of flame speed is only 0.34% when CURV = 0.06 and GRAD = 0.05. Those values satisfy the requirements of the present study. Thus the CURV = 0.06 and GRAD = 0.05 are used as a convergence setting in this study.

For the consideration of the intermediate species, the relevant species calculated from SENKIN are given in fig. 4. For the species which the mole fractions are extremely low are not considered, those species are represented by the nitrogen. In the calculation, EGR is cooled down to the initial temperature and EGR is considered as the complete combustion products H_2O, N_2, and CO_2. EGR ratio is calculated by:

$$\text{EGR [\%]} = \frac{n_{\text{EGR}}}{n_{\text{total}}} \cdot 100 \qquad (1)$$

Initial pressure of P_0 = 0.1 MPa, initial temperature of T_0 = 360 K, and equivalence ratio of 0.8 is chosen without EGR as the baseline condition for the comparison. The effects of initial pressure, initial temperature, equivalence ratio, and EGR ratio are studied, respectively. The effect of intermediate species is also investigated under all conditions.

Results and discussions

Effects of initial conditions on flame propagation

The effects of initial conditions including initial temperature, initial pressure, equivalence ratio and EGR ratio on flame propagation and HRR are shown in fig. 5. The effect of intermediates is also illustrated with and without intermediates. Flame speed and HRR under baseline condition of T_0 = 390 K, P_0 = 1.0 atm, ϕ = 0.8, and EGR = 0 is shown in fig. 5(a). The HRR of HCCI engine fueled with DME demonstrated a two-stage heat release, the LTHR with small heat release rate and the HTHR with large heat release rate [32] . With the increase of crank angle, the pressure and temperature increase due to compression and heat is released due to combustion. Flame speed increases monotonically with the increase of crank angle. Many researches have been conducted on the effect of pressure and temperature on flame speeds of various fuels under wide range of pressure and temperature conditions [33, 34]. The results showed that flame speed was increased with the increase of temperature and was decreased with the increase of pressure. The behavior in this study indicated that the flame speed determined by temperature rise due to compression and heat release from combustion with the increase of crank angle. The flame speed *vs.* crank angle can be classified into three regions. In the first region, flame speed increases slightly with the increase of crank angle. This region is close to the

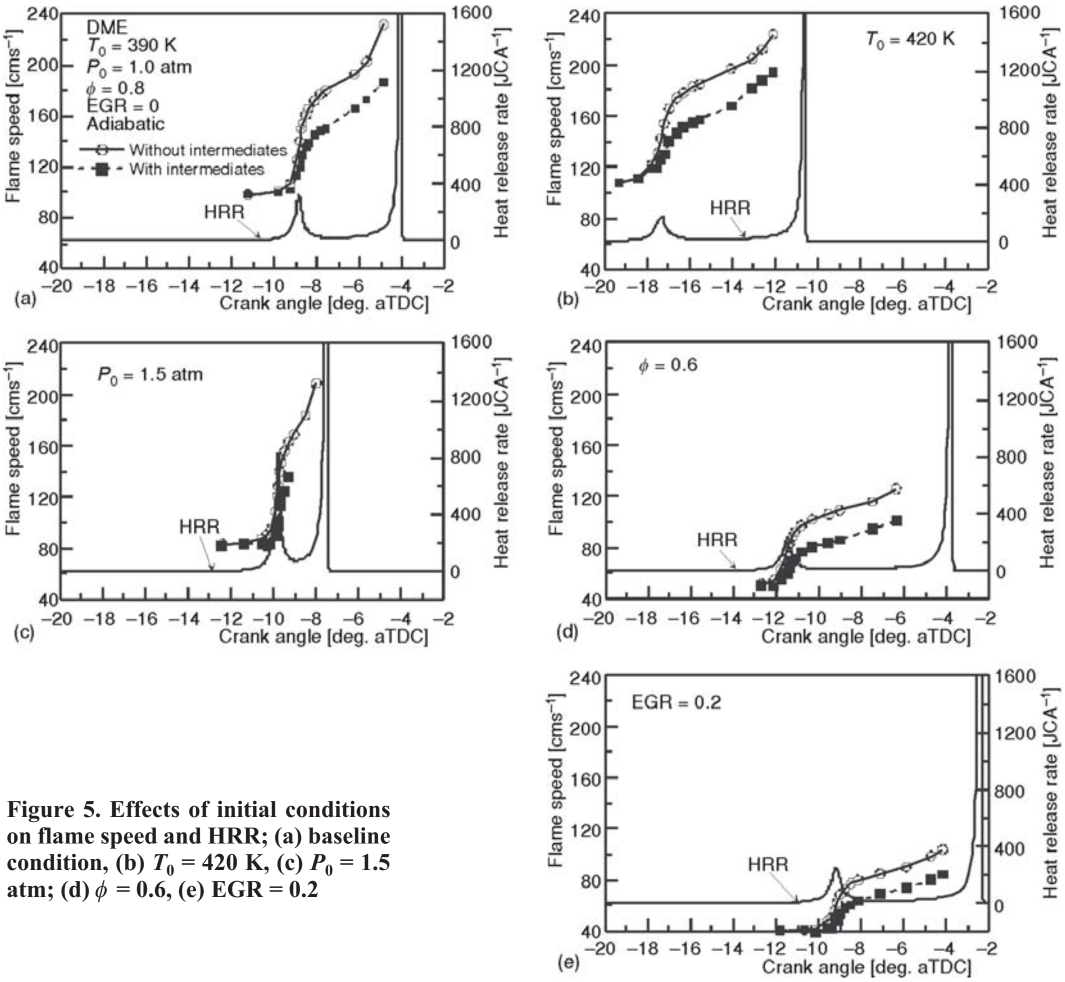

Figure 5. Effects of initial conditions on flame speed and HRR; (a) baseline condition, (b) T_0 = 420 K, (c) P_0 = 1.5 atm; (d) ϕ = 0.6, (e) EGR = 0.2

LTHR stage, where heat release is much limited. The increase of pressure and temperature is mainly resulted from the compression. The combined effect of pressure and temperature on flame speed leads to a little influence on flame speed with the increase of crank angle. The second region is from the start of LTHR to the end of LTHR, flame speed increases remarkably with the increase of crank angle. The LTHR of DME is cool flame reaction. Two-step oxidation of DME produces the OH radical and releases small portion of heat and increases the temperature and pressure [26]. The increase of temperature due to heat release causes a steep increase in flame speed. The third region is from the end of LTHR to the start of HTHR. Flame speed increases with the increase of crank angle. But the increase rate is lower than that of the second region. The temperature in this region is about 850 K to 1050 K. This region is called the NTC (negative temperature coefficient) region. During the NTC temperature range, the heat release is moderate to increase the temperature and prepare the bulk gas combustion. The rates of pressure and temperature rise decrease compared to the LTHR stage which slightly restricts the increase of flame speed.

The flame speed with intermediates is lower than that without intermediates and the difference between them is increased with the increase of crank angle after the LTHR stage. The intermediates species considered in this study are shown in fig. 4 and can be classified into three types. One is the triatomic molecules, H_2O and CO_2, which act as the dilution gas and will suppress the flame speed [35]. Another is the diatomic molecules, H_2 and CO. The last is the free radicals, OH, H_2O_2, HO_2, and CH_2O. The diatomic and free radicals will participate in the reaction and promote the flame speed. As shown in fig. 4, mole fractions of triatomic molecules, H_2O and CO_2 are much larger than other intermediates species. The dilution effect of triatomic molecules is the dominate effect of the intermediates on flame speed and suppresses the flame speed.

The effects of initial temperature and initial pressure on flame speed and HRR are given in figs. 5(b) and (c). Heat release is advanced and LTHR is suppressed at T_0 = 420 K compared to the baseline condition. Flame speed shows the similar tendency with the increase of crank angle. At initial pressure P_0 = 1.5 atm, the LTHR is promoted and heat release tends to be concentrated within a narrow crank angle range. The flame speed is slightly lower but increases much significantly compared to the baseline condition. The effect of equivalence ratio and EGR on flame speed and HRR is shown in figs. 5(d) and (e). The effect of equivalence ratio and EGR on flame speed and HRR is much similar as the mixture becomes the leaner with the decrease of equivalence ratio and the dilution with EGR. The phase of HRR postpones which leads to a smoother heat release in a real HCCI engine. However, flame speed decreases to half of the baseline condition and this decreases the proportion of the mixture consumed by flame propagation and the bulk mixture consumed by auto-ignition simultaneously. This indicates that the effect of equivalence ratio and EGR on flame propagation is much complicated and needs further investigation.

Combined effect of temperature and pressure on flame propagation

To understand the effect of temperature and pressure on flame propagation, the temperature, pressure, and HRR *vs*. crank angle under baseline condition of P_0 = 1.0 MPa, T_0 = 420 K, ϕ = 0.8, and *EGR* = 0 are given in fig. 6. The flame speed *vs*. temperature and pressure under baseline condition are given in fig. 7.

It can be seen that the temperature and pressure increased slightly with the increase of crank angle before the LTHR attributed to the compression. The temperature and pressure increased obviously after the LTHR due to the combustion heat release and the flame speed increased simultaneously. Figures 7(c) and (d) are the conditions of fig. 7(a) and (b) in the engine. It is seen from fig. 7(a) that the pressure of T_0 = 420 K is about 3.2 atm lower than that of baseline condition. The flame speed increased about 20 cm/s. However, it is seen from fig. 7(b) that the temperature of T_0 = 420 K is about 150 K higher compared to that at baseline condition which leads to the increase of about 70 cm/s higher in flame speed. This means that the flame speed in this study is mainly dominated by temperature rise due to the compression and heat release from combustion with the increase of crank angle, which is also discussed in fig. 5.

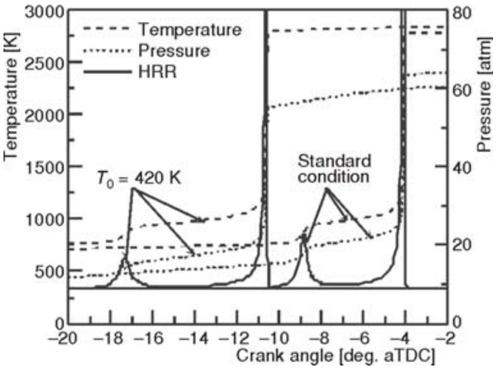

Figure 6. Temperature, pressure, HRR *vs*. crank angle

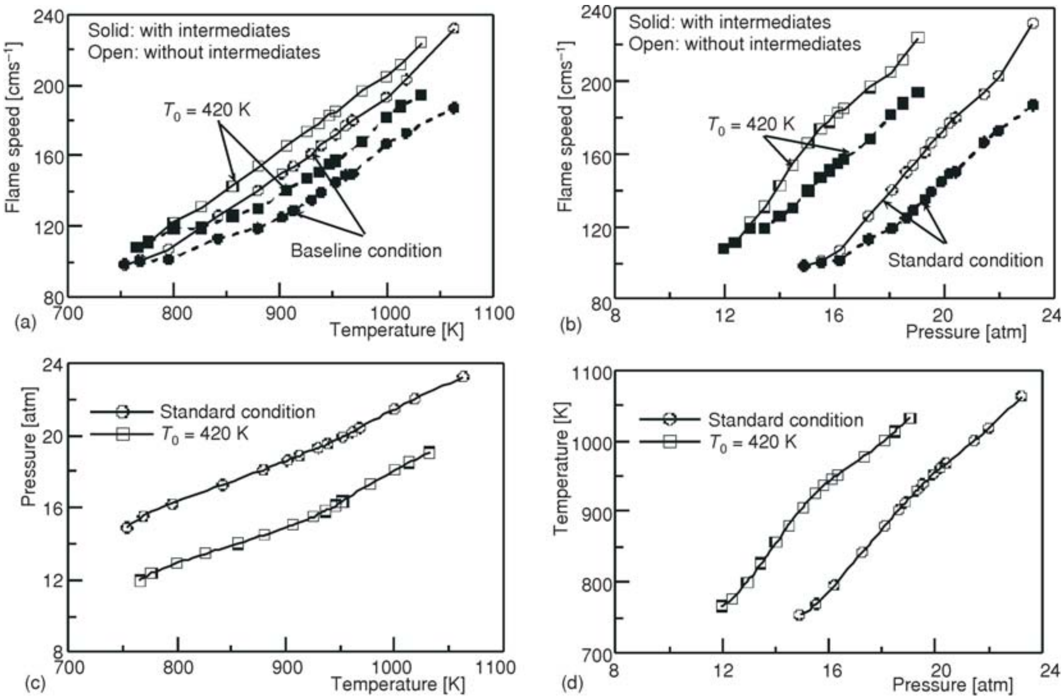

Figure 7. Combined effects of pressure and temperature on flame propagation: (a) and (c) flame speed and pressure *vs.* temperature; (b) and (d) flame speed and temperature *vs.* pressure

Conclusions

The flame propagation speed under various crank angles of a real HCCI engine was calculated. The effects of initial pressure, initial temperature, EGR ratio and intermediates on the flame propagation were investigated. Main results are as follows.

- Flame speed increases monotonically with the increase of crank angle, and it can be divided into a flat region, steep region and moderate increasing region.
- Effect of intermediates on flame propagation is mainly dominated by dilution effect which suppresses the flame propagation.
- Initial temperature and pressure just advance the crank angle of flame speed, but have little influence on its value. Equivalence ratio and EGR ratio not only distinctly decrease the flame speed but also advance the crank angle of flame speed.
- The flame speed in this study is mainly dominated by temperature rise due to the compression and heat release from combustion with the increase of crank angle.

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Nomenclature

DME – dimethyl ether

EGR – exhaust gas recirculation, [–]

HCCL – homogeneous charge compresion ignition
HTHR – high temperature heat release
HRR – heat release rate, [J/CA]
LTHR – low temperature heat release
NTC – negative temperature coefficient
P – pressure, [Pa]
PRF – primary reference fuel
PRR – pressure rise rate
P_0 – initial pressure, [Pa]
T_0 – initial temperature, [K]
ϕ – equivalence ratio, [–]

References

[1] Epping, K., *et al*., The Potential of HCCI Combustion for High Efficiency and Low Emissions, SAE technical paper 2002-01-1923, 2002
[2] Iida, N., Hyeonsook, Y., Combustion Research on Internal Combustion Engine Focus on Homogeneous Charge Compression Ignition, SAE technical paper 2009-32-0189, 2009
[3] Juttu, S., *et al*., Homogeneous Charge Compression Ignition (HCCI): A New Concept for Near Zero NO_x and Particulate Matter (PM) from Diesel Engine Combustion, The Automotive Research Association of India, SAE technical paper 2007-26-020, 2007
[4] Bogin, G. E., *et al.*, Homogeneous Charge Compression Ignition (HCCI) Engine, *SAE Int. J. Fuels Lubr., 2* (2009), 1, pp. 817-826
[5] Ghahfarokhi, R. F., *et al.*, Energy and Exergy Analyses of Homogeneous Charge Compression Ignition Engine, *Thermal Science, 17* (2013), 1, pp. 107-117
[6] Ying, W., *et al.*, Study of HCCI-DI Combustion and Emissions in a DME Engine, *Fuel, 88* (2009), 11, pp. 2255-2261
[7] Jung, D. W., *et al*., Influence of Pilot Injection on Combustion Characteristics and Emissions in a DI Diesel Engine Fueled with Diesel and DME, SAE technical paper 2011-01-1958, 2011
[8] Handford, D. I., Checkel, M. D., Extending the Load Range of a Natural Gas HCCI Engine using Direct Injected Pilot Charge and External EGR, SAE technical paper 2009-01-1884, 2009
[9] Gajarlawar, N., *et al*., Investigations of Effects of Pilot Injection with Charge in Level of Compression Ratio in a Common Rail Diesel Engine, *Thermal Science, 17* (2013), 1, pp. 71-80
[10] Odajima, R., *et al*., An Investigation of the Potential of EGR Stratification for Reducing Pressure Rise Rate in HCCI Combustion by Using Rapid Compression Machine, SAE technical paper 2011-01-1762, 2011
[11] Ozaki, J., Iida, N., Effect of Degree of Unmixedness on HCCI Combustion Based on Experiment and Numerical Analysis, SAE technical paper 2006-32-0046, 2006
[12] Sjöberg, M., Dec, J. E., Smoothing HCCI Heat-Release Rates Using Partial Fuel Stratification with Two-Stage Ignition Fuels, SAE technical paper 2006-01-0629, 2006
[13] Nakano, H., *et al*., An Investigation of the Effect of Thermal Stratification on HCCI Combustion by Using Rapid Compression Machine, Society of Automotive Engineers of Japan, SAE technical paper 2007-01-1870, 2007
[14] Naiki, T., *et al*., An Investigation of the Effects of Fuel Inhomogeneity on the Pressure Rise Rate in HCCI Engine Using Chemiluminescence Imaging, SAE technical paper 2010-32-0097, 2010
[15] Lü, X.-C., *et al*., Study on the Ignition, Combustion and Emissions of HCCI Combustion Engines Fueled with Primary Reference Fuels, SAE techical paper 2005-01-0155, 2005
[16] Saisirirat, P., *et al*., Effects of Ethanol, n-Butanol - n-Heptane Blended on Low Temperature Heat Release and HRR Phasing in Diesel-HCCI, Consiglio Nazionale delle Ricerche, SAE technical paper 2009-24-0094, 2009
[17] Machrafi, H., *et al.*, An Experimental and Numerical Analysis of the HCCI Auto-Ignition Process of Primary Reference Fuels, Toluene Reference Fuels and Diesel Fuel in an Engine, Varying the Engine Parameters, *Fuel Processing Tech, 89* (2008), 11, pp. 1007-1016
[18] Yao, M., *et al*., Effect of EGR on HCCI Combustion fuelled with Dimethyl Ether (DME) and Methanol Dual-Fuels, SAE technical paper 2005-01-3730, 2005
[19] Mack, J. H., *et al*., Investigation of HCCI Combustion of Diethyl Ether and Ethanol Mixtures Using Carbon 14 Tracing and Numerical Simulations, *Proc. Combust Inst, 30* (2005), 2, pp. 2693-2700
[20] Ohmura, T., *et al*., A Study on Combustion Control by Using Internal and External EGR for HCCI Engines Fuelled with DME, SAE technical paper 2006-32-0045, 2006
[21] Stuart Daw, C., *et al*., Understanding the Transition between Conventional Spark-Ignited Combustion and HCCI in a Gasoline Engine, *Proc. Combust. Inst, 31* (2007), 2, pp. 2887-2894

[22] Jung, D. W., Iida, N., A Computational Study of the Combined Effects of EGR and Boost Pressure on HCCI Autoignition, SAE technical paper 2012-32-0076, 2012
[23] Lim, O. T., *et al*., Experimental Study on HCCI Combustion Characteristics of n-Heptane and iso-Octane Fuel/Air Mixture by the use of a Rapid Compression Machine, SAE technical paper 2004-01-1968, 2004
[24] Jamsran, N., *et al*., An Investigation on DME HCCI Engine about Combustion Phase Control using EGR Stratification by Numerical Analysis, SAE technical paper 2012-32-0077, 2012
[25] Sato, S., Iida, N., Analysis of DME Homogeneous Charge Compression Ignition Combustion, Society of Automotive Engineers of Japan, SAE technical paper 2003-01-1825, 2003
[26] Yamada, H., *et al.*, Analysis of Reaction Mechanisms Controlling Cool and Thermal Flame with DME Fueled HCCI Engines, Society of Automotive Engineers of Japan, SAE technical paper 2006-01-3299, 2006
[27] Andrew, E., *et al*., A Fortran Program for Predicting Homogeneous Gas Phase Chemical Kinetics with Sensitivity Analysis, 1988
[28] Kee, R. J., *et al*., A Program for Modeling Steady, Laminar, One-Dimensional Premixed Flames, Sandia National Laboratories, Albuquerque, N. Mex., USA, 1985
[29] ***, CHEMKIN-PRO, Release 15112, Reaction Design, Inc., 2011
[30] Curran, H. J., *et al*., A Wide Range Modeling Study of Dimethyl Ether Oxidation, *Int. J. Chem Kinet, 30* (1998), 3, pp. 229-241
[31] Chen, G., *et al*., Numerical Study of EGR Effects on educing the Pressure Rise Rate of HCCI Engine Combustion, *Front. Energy Power Eng. China, 4* (2010), 3, pp. 376-385
[32] Kanehara, M., *et al*., Influence of Compression Speed on HCCI Ignition and Combustion, Society of Automotive Engineers of Japan, 2011-01-1779, 2011
[33] Daly, C. A., *et al*., Burning Velocities of Dimethyl Ether and Air, *Combust Flame, 125* (2001), 4, pp. 1329-1340
[34] Zhao, Z., *et al*., Measurements of Dimethyl Ether/Air Mixture Burning Velocities by Using Particle Image Velocimetry, *Combust Flame, 139* (2004), 1-2, pp. 52-60
[35] Chen, Z., *et al*., Experimental and Numerical Investigation on Diluted DME Flames: Thermal and Chemical kinetic Effects on Laminar Flame Speeds, *Fuel, 102* (2012), pp. 567-573

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