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Numerical Analysis of the Effect of Inhomogeneous Pre-Mixture on Pressure Rise Rate in HCCI Engine by Using Multi-Zone Chemical Kinetics

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1. Introduction

In HCCI, a premixed air/fuel mixture is inhaled to the combustion chamber and ignited by adiabatic compression. The HCCI engine, which is using the bulk combustion, is promising concept of the high efficient and low emission engine. However, power produced in HCCI engine is limited by knocking cause of excessive heat release and pressure rise at local area in condition of high load. Therefore, the main investigation of the HCCI is avoiding knocking problem to be able to operate at a high load. Delaying the combustion angle and stratifying temperature or concentration of fuel resulting in dispersion of combustion timing is the well-known effective method. In this study, effect of the pressure increase rate in combustion chamber by stratified temperature and fuel concentration of pre mixture according to fuel characteristic was investigated. Numerical analysis in chemical reaction was conducted for investigating an emission property.

2. Experimental method

In this paper, DME(Di-Methyle Ether) and Methane were used as a fuel. The Numerical analysis was conducted for the purpose of investigating that fuel or temperature stratification effect on pressure rise rate and emission using the multi-zone code with detailed chemical kinetics. DME has two stages of heat reaction which is called HTR(High Temperature Reaction) and LTR(Low Temperature Reaction). In case of DME, proportion of LTR is more than those of HTR. It is known that the more DME concentration make heat release increase during the LTR. Due to those facts, existing of DME fuel stratification in combustion chamber is expected to contribute reduction of gas pressure rise rate because heat release difference in local area during LTR causes stratification of temperature before the HTR which makes combustion duration extend. On the other hand, Methane has only 1 stage heat release and self-ignition temperature is high. The detailed specifications of the test engine are presented in Table 1. The hermetic gas is used for calculation duration from

Process	Only 1 Compression & Expansion
Bore X Stroke	112mm X 115mm
Displacement	1132cc
Length of Conrod	205mm
Crank Radius	57.5mm
Intake Valve Close Timing	ATDC-132
Exhaust Valve Open Timing	ATDC-132
Compresstion Ratio	8.0(DME)/21.6(Methane)

Table 1. Engine specifications

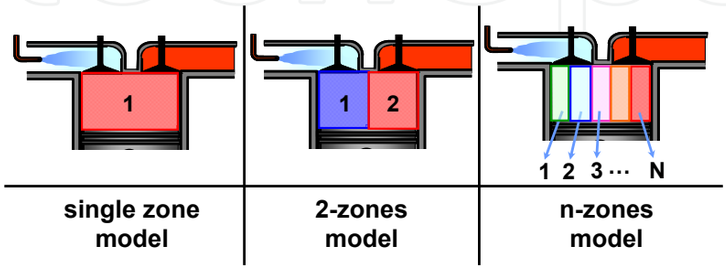


Fig. 1. Concept of multi-zone model

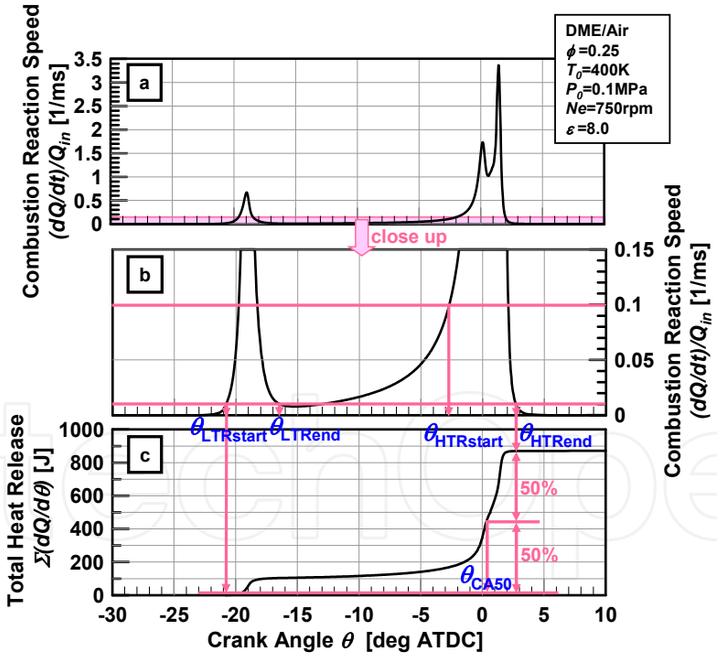


Fig. 2. Definitions of LTR start, LTR end, HTR start, HTR end and 50% heat release timing

the time that intake valve closed to the time that exhaust valve opened. As a calculation code, both CHEMKIN-II(5) and SENKIN(6) which is developed by Sandia National Laboratory is adjusted and then used. Curran for reaction of DME model, GRI-Mech3.0 for reaction of Methane model and Zeldvich for NOx model are used. The calculation is conducted following consumption. Heat loss and residual gas was neglected. All the

chemical gases were considered to be ideal gas and mass of pre mixture is assumed to be conservative. Multi-zone model is able to make stratification of temperature and fuel concentration in combustion chamber by changing the gas temperature and equivalent ratio before each of zones are compressed. Shown in Fig. 1, each zone model that is equally gas temperature and homogenous chemical species is 0-demension. Between the each zone, there is not chemical species and heat transfer but pressure is constant. The definition of CA50, start and end timing of both LTR and HTR are shown in Fig. 2 Shown in Fig. 2(a)(b), the combustion reaction velocity((dQ/dt)/Qin) was defined as rate of heat production divided by quantity of heat into the 1 cycle. Fig. 2(c) shows the integral hysteresis of heat production. The integral value of heat production rate from the LTR start to HTR end is consider 100% and then CA50 is defined 50% of heat production timing.

3. Analytical method

3.1 The effect of thermal stratification in pre mixture gas for reducing pressure rise rate

The calculation condition of equal equivalent ratio (Φ=0.25) and initial temperature T0 = 380K(Zone1), T1 = 420K(Zone2) using the DME/air and Methane/air is shown in Fig. 3, 4. The volumetric rate is changed to equalize the heat quantity into the each zone during 1 cycle. Gas pressure in combustion chamber, temperature and heat release rate in each of the zone by using the DME with fuel is shown in Fig. 5. Magnified LTR and HTR shown in

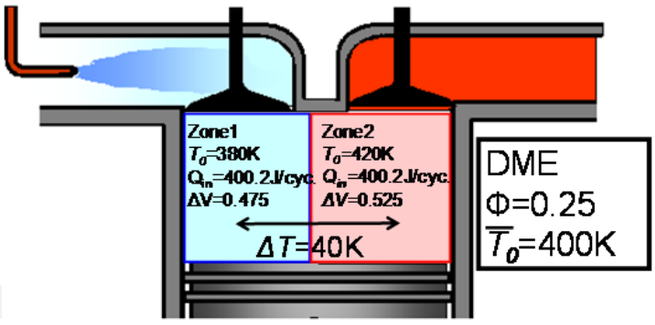


Fig. 3. Calculation condition (DME, Thermal stratification, 2-zones)

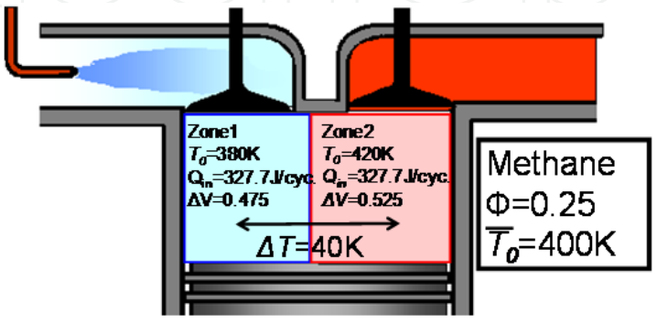


Fig. 4. Calculation condition (Methane, Thermal stratification, 2-zones)

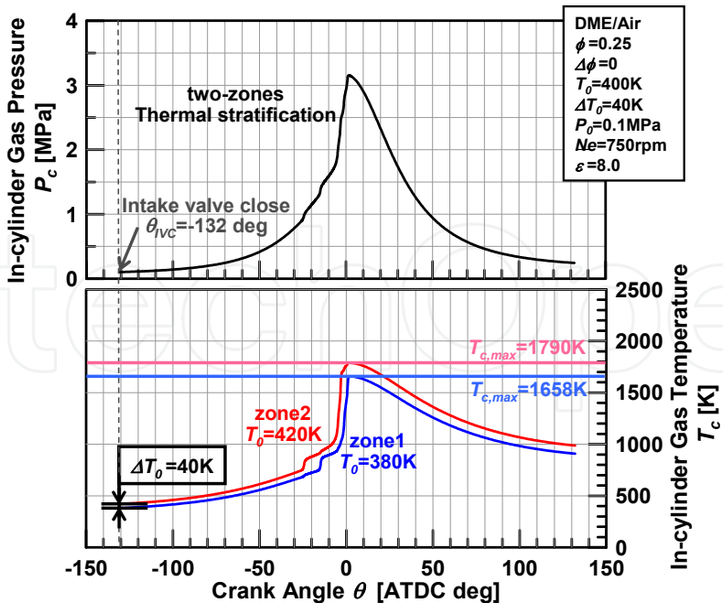


Fig. 5. Histories of in-cylinder gas pressure, in-cylinder gas temperature

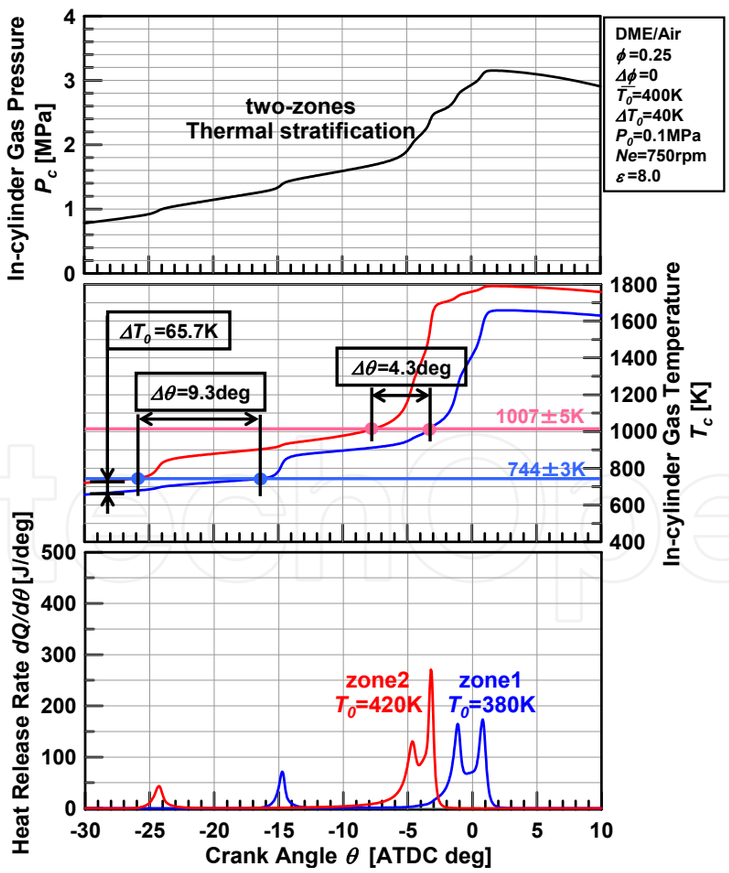


Fig. 6. Histories of in-cylinder gas pressure, in-cylinder gas temperature and heat release rate (DME, Thermal stratification, 2-zones)

Figure 6. First one is the graph of gas pressure in combustion chamber. Second and third one represent temperature and rat of heat release at each of the zone. LTR start temperature, HTR start temperature is almost constant as 744±3K, 1007±5K. Before LTR start, gas temperature difference in combustion chamber which is almost same as 40K according to piston rising is changed 65.7K before LTR start at zone 2. Because LTR start temperature is almost constant, LTR start is earlier about 9.3 deg at zone 2 than zone 1. Temperature difference between zone1 and zone2 is constant after LTR start so that HTR start is earlier about 4.3 deg than zone1. Also, using the fuel as a Methane, gas pressure in combustion chamber, temperature and heat release rate in each zone is shown in Fig. 7. The temperature of HTR start is 1177± 3K. Zone 2 with higher temperature than zone1, HTR start is earlier about 4.5deg than zone 1 before the compression stroke by using the Methane as a fuel.

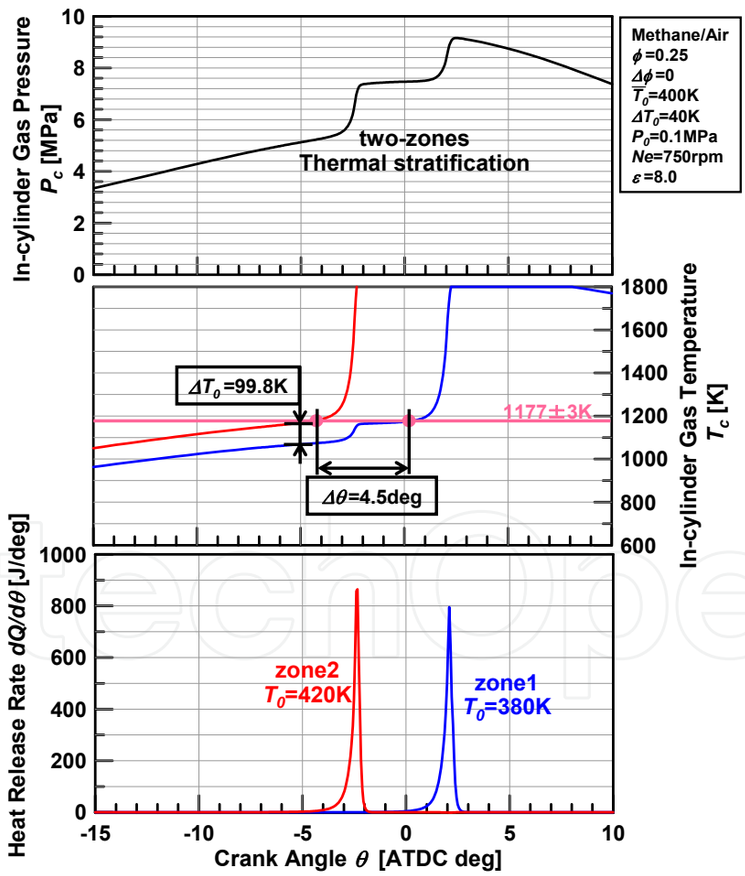


Fig. 7. Histories of in-cylinder gas pressure, in-cylinder gas temperature and heat release rate (Methane, Thermal stratification, 2-zones)

3.2 The effect of fuel stratification in pre mixture gas for reducing pressure rise rate

At the beginning of compression, the average gas temperature (T0 = 400K) is assumed. The calculation condition is shown in Fig. 8, 9 that is Φ = 0.17(zone1) Φ= 0.47(zone2) in each of the zone using the Methane or DME. Gas pressure in combustion chamber, gas temperature and rate of heat release in each of zone are shown in Fig. 10. Magnified graph was shown in Fig. 11. Temperature of LTR start and HTR start is 747±3 K, 1009±1. Temperature difference in combustion chamber is getting bigger according to piston rising before the LTR start due to difference of specific heat caused by equivalent ratio and temperature rising rate. Temperature difference before the compression stroke is changed from 0K to 17.3K before LTR start in zone1. LTR start is earlier at zone 2 about 2.3deg. However, Large amount of heat release during LTR in higher equivalent ration zone make trace of gas temperature be reversed in zone2 when LTR end. Due to gas temperature reversing, HTR start is earlier about 2.3 deg in zone 2 than zone1. Gas pressure in combustion chamber, gas temperature and heat release rate in each of the zone is shown in Fig. 12. HTR start temperature is 1163±11 K. Similar with DME, the Methane gas temperature difference in combustion chamber is getting big according to piston rising. However, Methane doesn't have LTR but 1 stage of heat release. So it can be expected HTR start in zone2 is later than zone 1 about 3.1 because of lean concentration of zone 1.

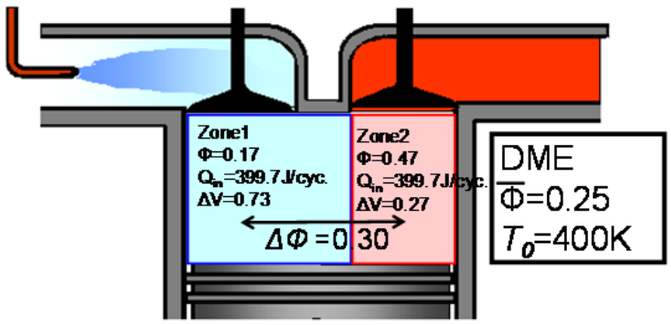


Fig. 8. Calculation condition (DME, Fuel stratification, 2-zones)

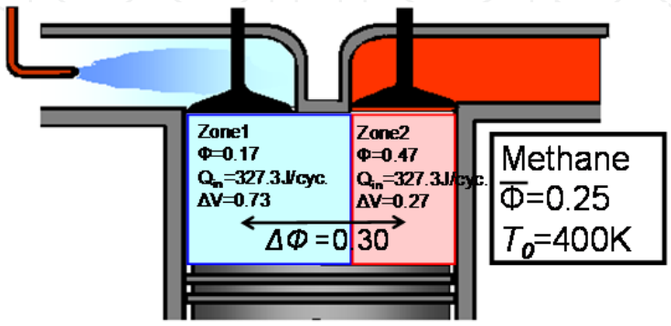


Fig. 9. Calculation condition (Methane, Fuel stratification, 2-zones)

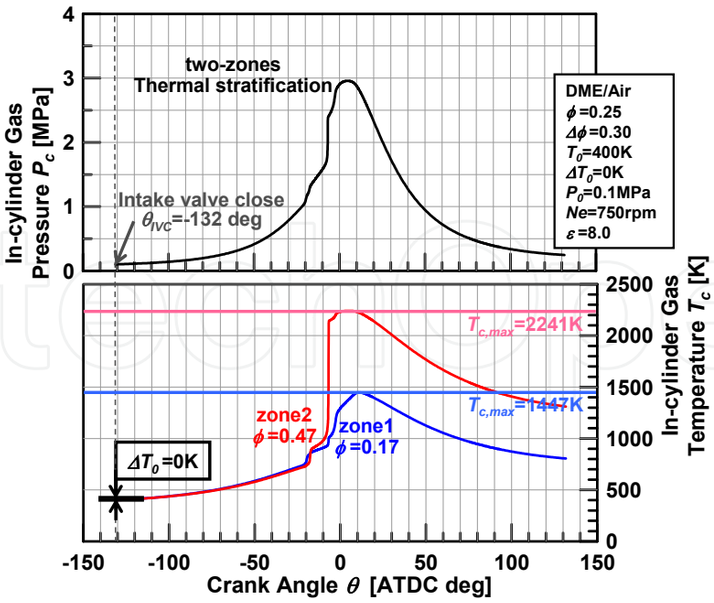


Fig. 10. Histories of in-cylinder gas pressure and in-cylinder gas temperature (DME, Fuel stratification, 2-zones)

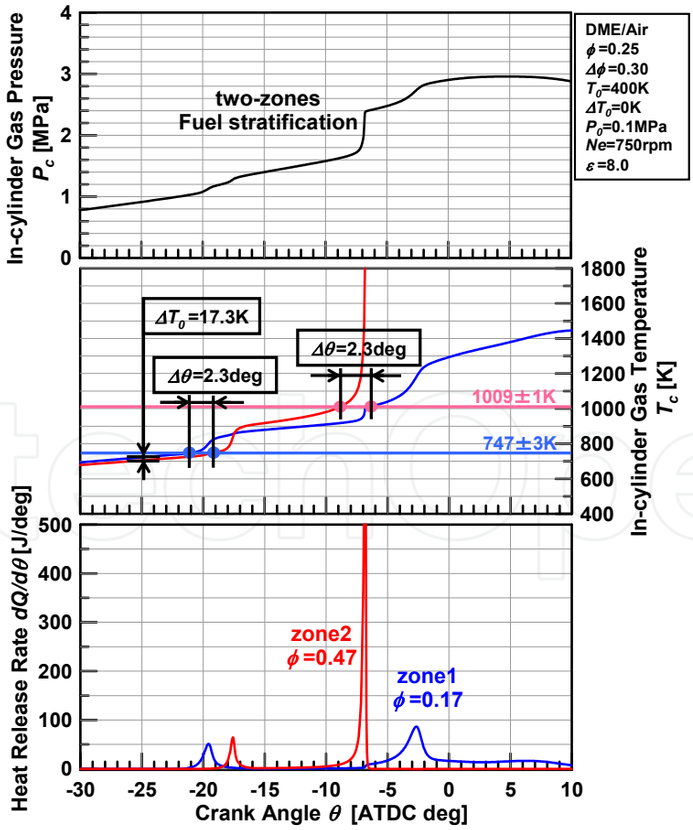


Fig. 11. Histories of in-cylinder gas pressure, in-cylinder gas temperature and heat release rate (DME, Fuel stratification, 2-zones)

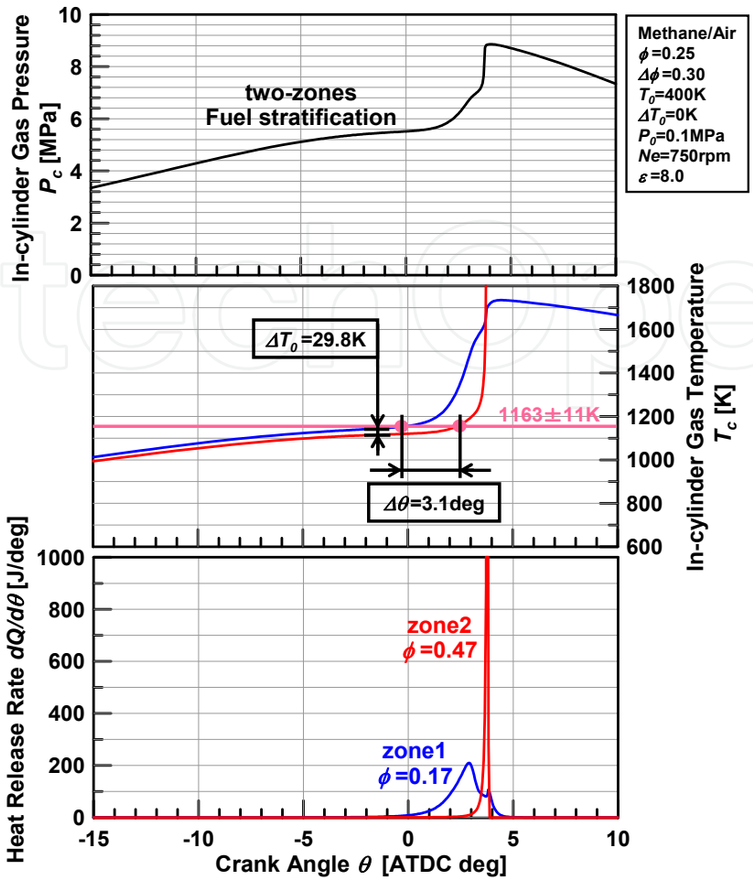


Fig. 12. Histories of in-cylinder gas pressure, in-cylinder gas temperature and heat release rate (Methane, Fuel stratification, 2-zones)

4. Results and discussion

4.1 Analysis of reducing maximum pressure rising rate effect and emission feature by multi-zone

Based on result of 2-zone model, reducing gas pressure rate, heat release and emission is investigated in combustion chamber when there is more temperature and fuel distribution by using the numerical analysis at 5 model-zone to expand and vary the stratification. Using the DME and Methane, the relation between CA50% and maximum pressure rise rate is shown in Fig..13-16 in condition of average equivalent ratio(φ=0,25) and changing the average temperature before the compression from T0=300K to T0=500K. In terms of temperature stratification, 5K average pre mixed gas temperature difference was given between each zone before compression and computation calculation was conducted in condition of T0=20K and T0=40K between highest and lowest zone. On the other hand, in terms of concentration stratification, average equivalent ratio(φ=0.25) is set up and computation calculation was conducted in condition of Δφ=0.10 and Δφ=0.30 between highest and lowest zone. Afterward, this result is compared with condition of equal temperature and concentration of pre-mixture gas. Comparing the result of temperature difference and concentration in pre-mixed gas, without any relation on amount of

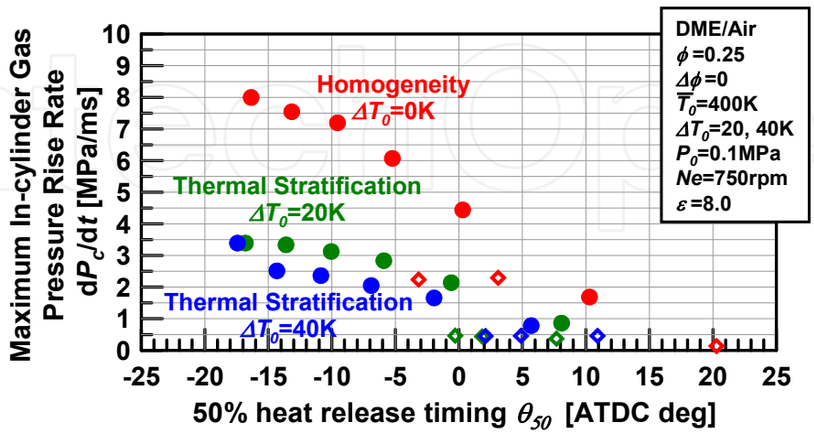


Fig. 13. 50% heat release timing and maximum in-cylinder gas pressure rise rate (DME, Thermal stratification, 5-zone)

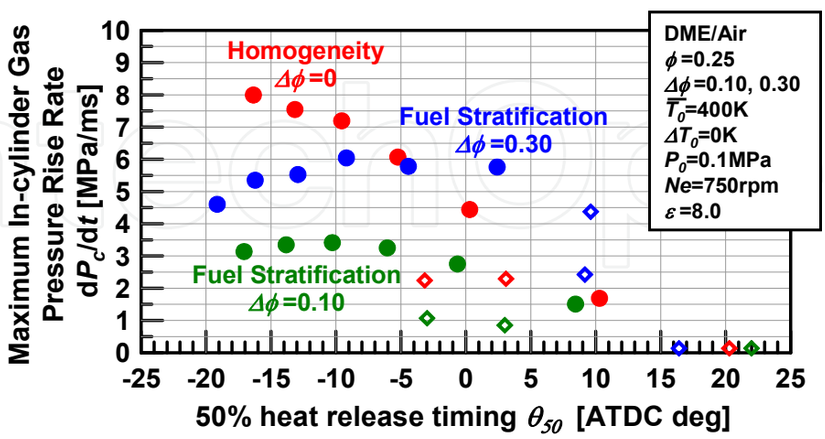


Fig. 14. 50% heat release timing and maximum in-cylinder gas pressure rise rate (DME, Fuel stratification, 5-zone)

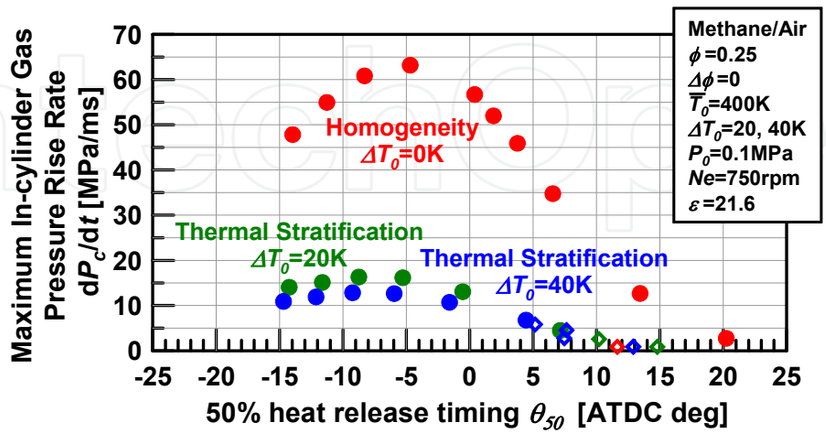


Fig. 15. 50% heat release timing and maximum in-cylinder gas pressure rise rate (Methane, Thermal stratification, 5-zone)

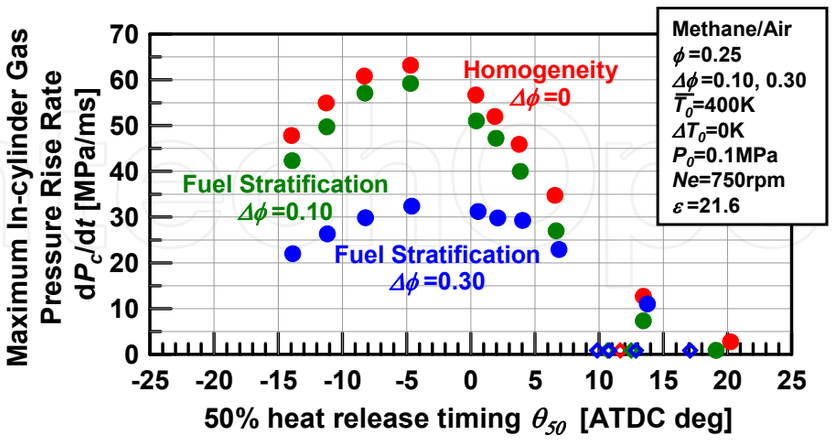


Fig. 16. 50% heat release timing and maximum in-cylinder gas pressure rise rate (Methane, Fuel stratification, 5-zone)

temperature difference, the maximum pressure rise rate is reduced below 50% beside homogeneous pre-mixed gas. The reduce rate is getting big, temperature difference is more. Its decrease rate is changed in a rage of concentration largely although the maximum pressure rise rate is reduced compared with homogenous pre-mixed gas when there is density difference. The rage of concentration which obtained reducing maximum pressure rise rate result is different comparing between DME and Methane. It can be expected that obtained result is different between DME and methane. The reason is that temperature difference by the piston compression before the LTR is disappeared and gas temperature trace is reversed at LTR end due to LTR existing in DME. In condition of 400K gas average temperature before the compression (T0), NOx, CO concentration in emission, combustion efficiency and maximum temperature in combustion chamber is shown in Fig. 17-20. The effect of temperature and concentration stratification on the emission characteristic was discussed by comparing pre-mixed gas with stratified temperature and concentration condition and equal temperature and concentration condition as T0=400K, equivalent ratio=0.25. Concentration of CO is increased bellow 1500K maximum temperature and NOx concentration is increased above 2100K. NOx and CO in emission gas concentration is almost same comparing the equal pre-mixed gas because maximum temperature is between 1500K and 2100K in each zone using DME and Methane existing temperature stratification in pre-mixed gas. NOx, CO concentration is getting big comparing with equal pre-mixed gas in emission gas because maximum temperature is above 2100K with high equivalent ratio in condition of concentration stratification.

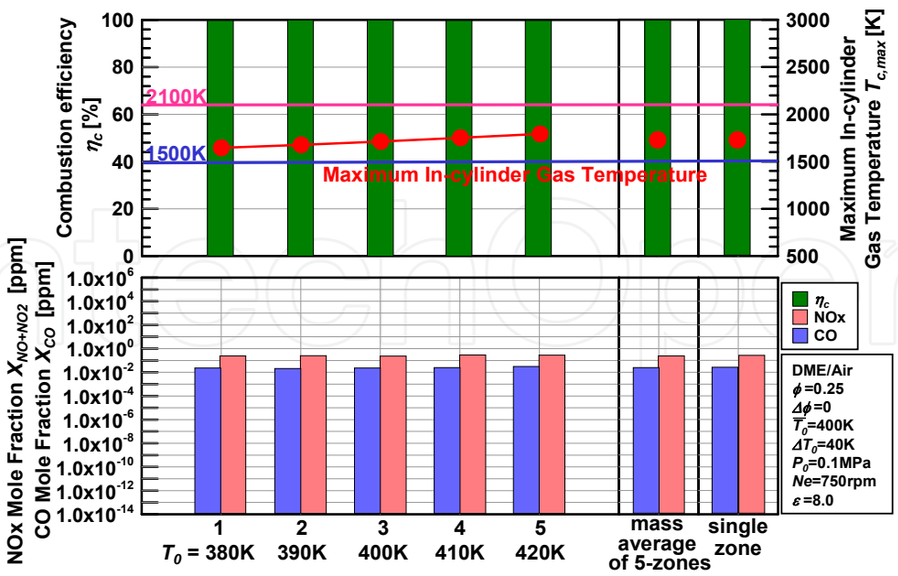


Fig. 17. CO and NOx mole fraction in exhaust gas, combustion efficiency and maximum in-cylinder gas temperature (DME, Thermal stratification, 5-zones)

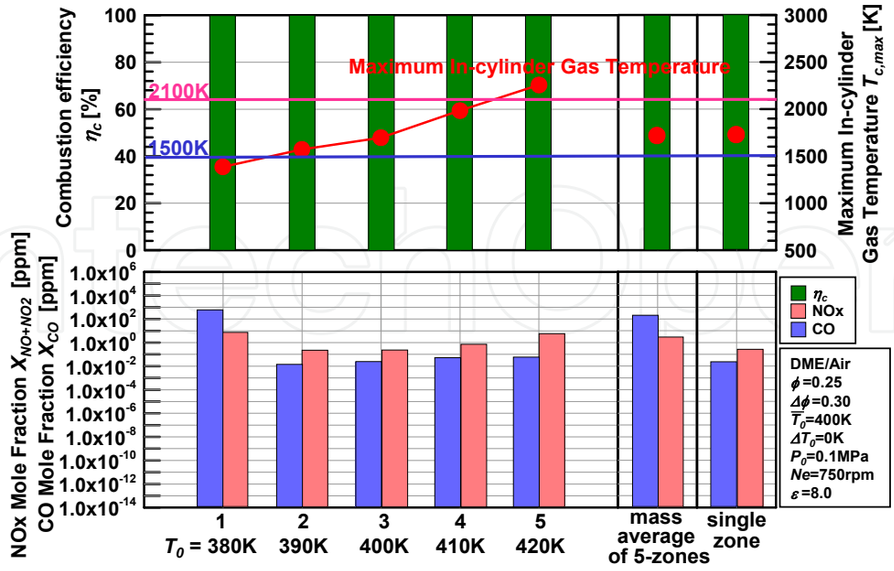


Fig. 18. CO and NOx mole fraction in exhaust gas, combustion efficiency and maximum in-cylinder gas temperature (DME, Fuel stratification, 5-zones)

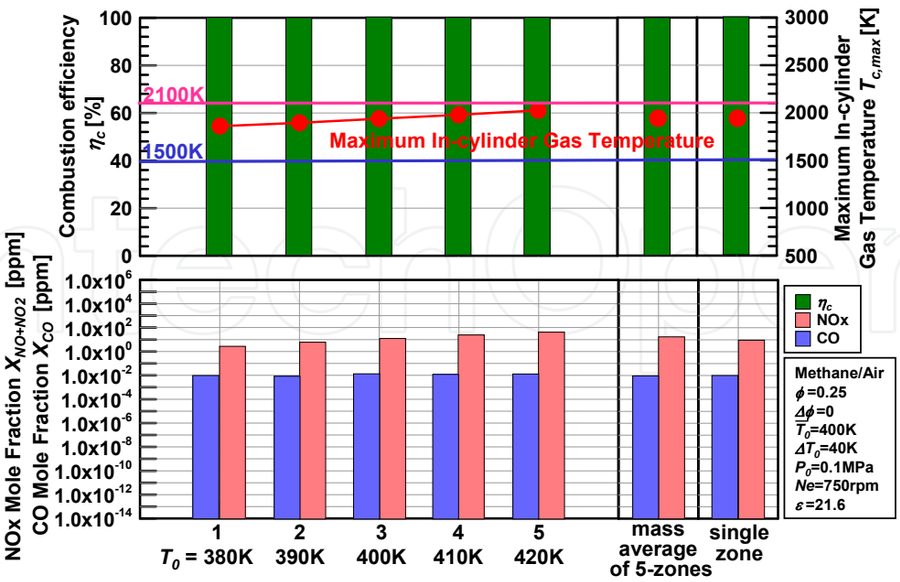


Fig. 19. CO and NOx mole fraction in exhaust gas, combustion efficiency and maximum in-cylinder gas temperature (Methane, Thermal stratification, 5-zones)

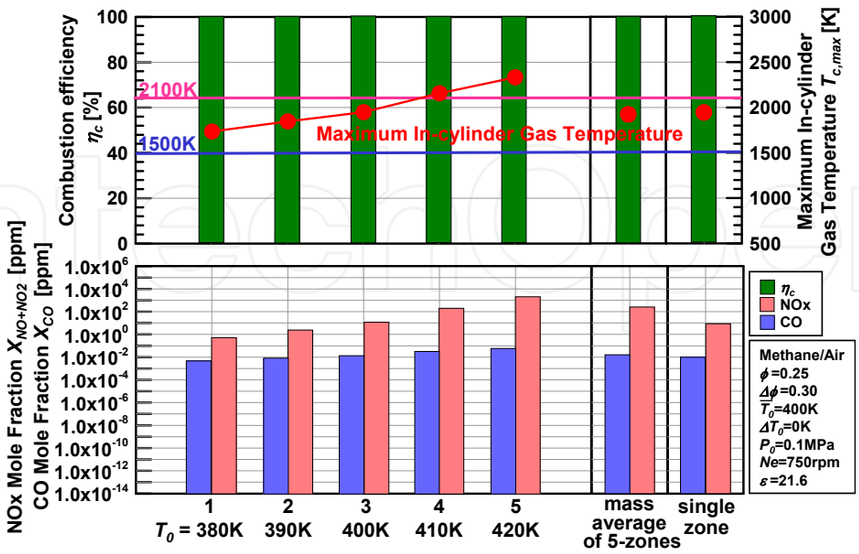


Fig. 20. CO and NOx mole fraction in exhaust gas, combustion efficiency and maximum in-cylinder gas temperature (Methane, Fuel stratification, 5-zones)

5. Conclusion

Chemical reaction numerical computation was conducted by giving a temperature or concentration stratification to pre-mixture. The reducing pressure rise rate effect is investigated by temperature and concentration stratification in pre-mixture. Choosing the DME and Methane that heat release characteristic is different, using the detailed reaction scheme and conducting numerical computation in multi-zone, following knowledge is affordable.

1. In condition of stratified temperature pre-mixture, temperature difference of the combustion chamber is expanded by piston compression. LTR or HTR occur earlier at the zone that gas temperature is higher.
2. In condition of stratified fuel pre-mixture, temperature difference of the combustion chamber is occurred. LTR is occurred earlier in the zone which is lower concentration beside HTR is opposite.
3. In condition of stratified temperature and concentration, maximum pressure rise rate is decreased largely as compared with equal condition. Especially, maximum pressure rise rate is reduced restricting NOx, CO emission amount in condition of stratified temperature which is same as equal condition.
4. Concentrate stratification control is needed to operate the engine between 1500K and 2100K in condition of stratified concentration in pre-mixture.
5. Optimized succeeding investigation what temperature and concentration of stratification is most efficient is needed to reduce both maximum pressure rise rate and emission together efficiently

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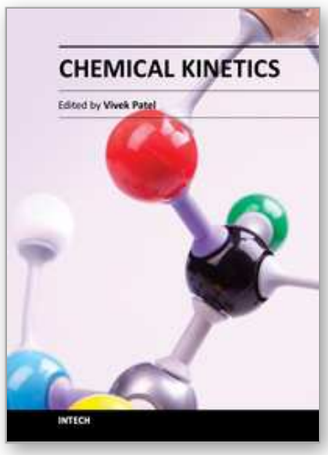
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Chemical Kinetics relates to the rates of chemical reactions and factors such as concentration and temperature, which affects the rates of chemical reactions. Such studies are important in providing essential evidence as to the mechanisms of chemical processes. The book is designed to help the reader, particularly students and researchers of physical science, understand the chemical kinetics mechanics and chemical reactions. The selection of topics addressed and the examples, tables and graphs used to illustrate them are governed, to a large extent, by the fact that this book is aimed primarily at physical science (mainly chemistry) technologists. Undoubtedly, this book contains "must read" materials for students, engineers, and researchers working in the chemistry and chemical kinetics area. This book provides valuable insight into the mechanisms and chemical reactions. It is written in concise, self-explanatory and informative manner by a world class scientists in the field.

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