DIESEL/METHANOL DUAL FUELS COMBUSTION- A MODE CONTROLLED BY BOTH CHEMICAL KINETIC AND PHYSICAL PROCESS

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Summary. The diesel/methanol dual fuel combustion mode is that diesel fuel spray penetrates into hot methanol/air ambient and then premixed methanol is ignited in C.I. engine. There are three zones in the combustion, i.e. the diesel fuel rich zone, premixed methanol zone and diesel mixed with methanol zone respectively. The aim of this work is focused on investigations into the behaviour of the dual fuel combustion comprehensively especially the chemical kinetics involve the fuels oxidation and the formation of the soot precursors.

INTRODUCTION

The dual fuels combustion applied on compression ignition engine has some excellent advantage such as the on line flexible fuel design to achieve PCCI or LTC combustion mode and getting rid of dependence on petrol. Generally dual fuel combustion is the fuel with high cetane number injected into the mixture of air and the fuel with high octane number. Most engine bench test and in-cylinder simulation results show that low emission and high efficiency can be achieved by this mode [1]. In this conception, the chemical kinetic becomes more important than conventional combustion. However by contrast with most single fuels, the interaction between the fuels which have substantially different combustion behaviours is still under study. In this work, methanol as a simple fuel with high octane number and n-heptane as well as toluene which are common component in surrogate of petrol fuels is adopted in their co-oxidation study. The research topic is mainly focus on high temperature oxidation.

CONCEPTION

The combustion mode of methanol-air mixture ignited by diesel is more complex since it involves the diffusion flame in C.I. engine and the flame propagation in S.I. engine. Fig. 1 shows the fuel distribution before ignition. The combustion chamber can be divided into three zones: Zone A is the fuel rich zone in the spray centre, which is filled with diesel and a small amount of methanol. The concentration of methanol in this zone is higher than the surround zone because of the entertainment effect of spray. After ignition, it is the major soot generation zone just as conventional C.I. engine. The chemical kinetic including soot formation between alcohol and hydrocarbons will be studied in this work; Zone B is the premixed zone of methanol/air mixture. The oxidation behaviours involve flame propagation as what happened in conventional S.I. engine, the auto-ignition of methanol (knock) and NO formation at the flame front. By the way, formaldehyde and CO are mainly generated in the squish and crevice which are also a part of zone B. So both chemical kinetics of the premixed fuel and the turbulence interaction must be paid attention. Zone C is a critical area of both fuel and air mixture with appropriate equivalence ratio. It is different form conventional C.I. engine or S.I. engine since the couple relation mainly occurs in this regain, which is hydrocarbon fuel diffusing into alcohol fuel/air mixture. The ignition is determined by the formation of this region. Several factors such as temperature, mixing ratio, equivalence ratio and diffusion rate can control the ignition delay. After ignition, physical mixing will take over the chemical factor to be the main factor. High temperature oxidation will also control the NO and part of soot formation.

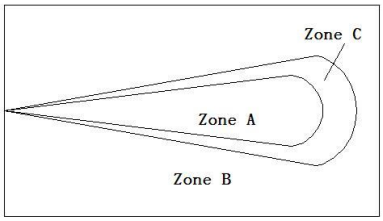

Fig. 1 Zones divided in diesel/methanol combustion mode

CHEMICAL KINETICS

Chemical kinetic is more important than physical factor in this combustion since it the couple relationship between the fuels can mainly be attributed to the molecular level. First, the ignition property of n-heptane and methanol is totally different, and the couple relationship between them has been studied detailed in our previous work [2], here in brief: The reaction path analysis shows that the radical pool is the only bridge connecting the two fuels in the low temperature oxidation, and the direct couple relationship between the large fuel molecules can be neglected. At the first stage, both fuels undergoes the H abstraction by an OH radical, two OH radicals will be returned by the chain-

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branch reaction of n-heptane next, however no activity radical can be generated by the methanol oxidation immediately. So methanol is the role which converts activity OH into inactivity H_2O_2. The latter then is accumulated into a large amount and decomposes suddenly when the temperature exceeding about 1000K. So the reactivity of the whole system decreases.

In the high temperature oxidation study, low pressure laminar premixed flame combining with synchrotron radiation TOF-MS detection technology [3] is adopted. Toluene as an aromatic hydrocarbon was added into the fuel mixture in order to simulate the soot formation properties of diesel. The detailed mechanism is build based on USC Mech II [4]. In this study, both methanol and ethanol were used for experimental and detailed mechanism modelling comparison study. The high temperature oxidation sub-mechanism in our previous skeletal model [2] is established based on the assumption of n-heptane and methanol has no relationship in the temperature above 1200K. The results in this study shows that the decomposition reactions of n-heptane and toluene are not affected by alcohol addition, the decreases of the mole fractions of alkene and benzene is attributed to the decreases of the initial mole fraction of hydrocarbon fuels (See Fig. 2 as an example). So the assumption is confirmed. However the mole fraction of the growth products such as the PAH shows that with the degree of unsaturation increasing, the reducing effect for the mole fraction of hydrocarbon intermediate by alcohol addition becomes obviously (See Fig. 3 as an example). In addition, other species with low molecular weight such as C_4H_6 to C_4H_2 also has the same behaviours except PAH. This work is still underway, so the high temperature oxidation of n-heptane and methanol in the skeletal model mentioned above does not include the soot reactions yet.

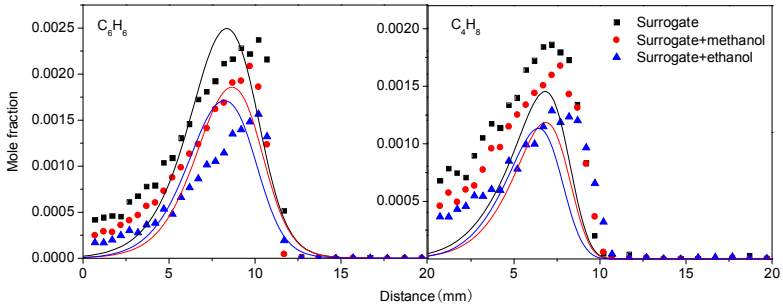

Fig. 2 mole fraction of butane and benzene

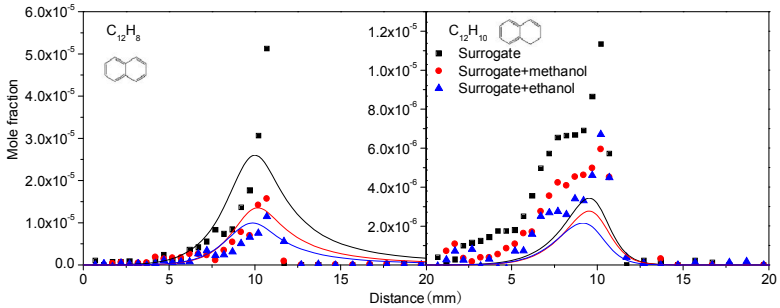

Fig. 3 Mole fraction of C_{12} aromatic hydrocarbons

CONCLUSIONS

Several factors especially the chemical kinetic in diesel-methanol dual fuels combustion are studied in this work. Three zones can be divided in the combustion chamber, they are the diesel/methanol fuel rich zone, methanol premixed zone and the critical zone. Each zone has its own oxidation property including auto-ignition, high temperature combustion, PAH formation and flame propagation. It has been cleared that methanol has a destruction effect on OH below about 1000K to inhibit the ignition of n-heptane in low temperature oxidation. But the decompositions of alcohol and hydrocarbon are confirmed to have no relationship in high temperature low pressure premixed laminar flame. However alcohol has an effect on the decrease of PAH mole fraction. With the degree of unsaturation increase, this effect becomes obviously.

Acknowledgement

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