Investigation on Combustion Characteristics of Methanol-Syngas Fuel

Yexin Chen* and Yankun Jiang*

School of Energy and Power Engineering, Huazhong University of Science and Technology, Wuhan, China

*Corresponding author e-mail: jykhust@hust.edu.cn, *chenyexin@hust.edu.cn

Abstract. Methanol has a broad application prospect in internal combustion engine due to its renewable and environment-friendly characteristics. In this research, a method of using mixture of methanol and syngas as internal combustion engine fuel is proposed, while the syngas is produced by dissociating the methanol through making use of the exhaust heat of the engine. By analyzing reaction path of fuel oxidation and sensitivity analysis of elementary reactions, the effect of syngas on the oxidation process of fuel was studied. The effect of blending ratio and equivalence ratio on ignition delay time and laminar flame speed was investigated. The research results can provide theoretical guidance for the application of methanol-syngas fuel in internal combustion engine.

1. Introduction

Methanol (CH$_3$OH) is one of alternatives to fossil fuels that can avoid a net carbon emission and can decrease pollutant emissions [1]. When methanol is used as vehicle fuel, we can dissociate part of methanol into hydrogen (H$_2$) and carbon monoxide (CO) by exhaust heat, which can make full use of the exhaust heat, change the combustion characteristics of the fuel to further improve the efficiency and reduce emission of the internal combustion engine, as shown in Figure 1.

![Figure 1. Schematic diagram of methanol-syngas engine concept](Image)

Ji, Gong and Nguyen have made research on the application of mixture fuel of methanol-hydrogen and mixture fuel of methanol-reformed gas. Research results show that hydrogen can reduce the emissions of unburned hydrocarbons and CO, and increase the efficiency of fuel [2-3]. The knock limit for spark-ignited operation is extended with rising dilution level [4].

Content from this work may be used under the terms of the Creative Commons Attribution 3.0 licence. Any further distribution of this work must maintain attribution to the author(s) and the title of the work, journal citation and DOI. Published under licence by IOP Publishing Ltd
Burke have developed the methanol combustion mechanism which can be applied for a wide range of conditions. The accuracy of the mechanism has been demonstrated by shock tube, rapid compression machine, jet-stirred reactor, and other experimental verification. Mechanism proposed by Burke is used for combustion characteristics research in this paper [5].

To sum up, the combustion of H\textsubscript{2}-containing Syngas can significantly improve the engine efficiency and reduce emissions. According to research, the addition of hydrogen can increase flame speed, widen lean burn combustion limit. However, the composition of methanol dissociated gas is different and more complex than that of hydrogen, and the characteristics of methanol-syngas fuel have not been involved in the present research. Therefore, in this research, the combustion characteristics of methanol-syngas fuel were investigated, the syngas is produced by dissociating the methanol and its composition is 66.67% H\textsubscript{2} and 33.33% CO in mole fraction.

2. Oxidation process of methanol-syngas fuel
This research analyses the oxidation process of CH\textsubscript{3}OH, H\textsubscript{2} and CO in methanol-syngas mixed fuel. As is shown in Figure 2(a). In the oxidation process of fuel, methanol is firstly oxidized, and its direct product is CH\textsubscript{2}OH and CH\textsubscript{3}O, but these two are unstable radicals, and then the stable CH\textsubscript{2}O is produced rapidly. In the subsequent combustion phase, CH\textsubscript{2}O is oxidized to HCO, which is rapidly converted to CO, and when CO is oxidized to CO\textsubscript{2}, a great deal of heat is released meanwhile. Both CH\textsubscript{3}OH and CH\textsubscript{2}O may produce H\textsubscript{2} during dehydrogenation reaction with H\textsubscript{2} radical.

![Figure 2](image_url)

**Figure 2.** (a) Reaction path analysis and (b) sensitivity analysis of methanol-syngas fuel

In this research, the sensitivity analysis on elementary reactions of different blending ratio was conducted, as figure 2(b) shown. The blending ratio was separately 0%, 10%, 50%, equivalence ratio was 1, temperature was 1000K, pressure was 30atm. The results in figure 2(b) show sets of elementary reactions with the highest sensitivity.

R21 is the most important chain branching reaction. Its product OH will participate in other subsequent reactions, so the speed of this reaction can affect the overall reaction rate significantly. R121, R122 and R123 are dehydrogenation of methanol, which are three chain starting reactions. They largely controls the concentration of reactants in following steps. The product of R123 is reactant for the chain branching reaction of R21, so its reaction rate has the greatest influence on the overall reaction. The reaction rate of R122 is much slower than that of R123 because the H on methyl radicals is easier to detach compared with H on hydroxyl radicals. The products of R157 are also relatively important because it is the reactant in chain branching reactions of R21. In the R32 reaction, the reactants contain...
two radicals, while the products have only one radical, which is a chain termination reaction, such reaction will reduce the overall reaction rate, so the sensitivity coefficient is negative.

In general, the absolute sensitivity of the overall reaction rate increases with the increase of the blending ratio. Regarding R3 and R23 reactions, H₂ have little effect on the overall reaction rate at low blending ratio, but the effect at high blending ratio can not be neglected.

3. Ignition delay time analysis of methanol-syngas fuel

Ignition delay time is a factor that must be considered in the design of internal combustion engine. In this study, the effects of different blending ratios and different equivalence ratios on the ignition delay time were investigated, as shown in Figure 3. The temperature range is 1000K-1450K, the pressure is 30atm, the dilution rate is 80% and Ar is used. The results show that the relationship between the ignition delay time and the temperature is in good agreement with Arrhenius equation.

![Figure 3. Ignition delay time of fuel at (a) different blending ratios and (b) different equivalence ratios](image)

In the figure 3(a), the blending ratios were 0%, 10% and 50% respectively, and the equivalence ratio was 1. It can be seen from the diagram that the ignition delay time is prolonged with the increase of the blending ratio. The main reason is that the dehydrogenation of methanol to produce radical is faster than the decomposition of hydrogen molecules to produce radicals at the initial stage of fuel oxidation. On one hand, the addition of syngas reduces the concentration of methanol molecules in the fuel. On the other hand, hydrogen molecules compete with methanol molecules for the radicals, these are the reasons why the ignition delay time increases with the increase of syngas blending.

In the figure 3(b), the equivalence ratios are 0.5, 1.0 and 1.2 respectively, and syngas blending ratio is 50%. With the addition of syngas, the lean combustion limit of the fuel has been extended, even 0.5 equivalence ratio can catch fire normally. From the results of analysis, it can be seen that the ignition delay time shortens with the increase of the equivalence ratio because the concentration of fuel molecules increases. This increases the collision probability of the fuel molecules with oxygen molecules and intermediate products, in other words, increases the reaction rate, thus shortening the ignition delay time.

4. Laminar flame speed analysis of methanol-syngas fuel

The laminar flame speed has an important influence on the timeliness of combustion and the thermal efficiency of internal combustion engine. This research analyses the influence of different blending ratios and different equivalence ratios on the flame speed. The studies are conducted on a typical spark ignition engine relevant condition, temperature of 700K and pressure of 20atm.

As can be seen from figure 4(a), flame speed increases with the increase of the blending ratio. This is due to the fact that the flame speed of hydrogen is much faster than that of methanol. The maximum
flame speed appears when the equivalence ratio is slightly greater than 1. With the increase of the blending ratio, the equivalence ratio of the maximum flame speed increases.

![Figure 4. Flame speed of fuel at (a) different equivalence ratios and (b) different blending ratios.](image)

Figure 4(b) clearly reflects the increase of flame speed with the increase of blending ratio. When the blending ratio is less than 50%, the flame speed increases slowly with the increase of the blending ratio, and when the blending ratio is more than 50%, the flame speed increases faster and faster, it also accords with the phenomenon that the flame speed increases with the increase of the equivalence ratio when the equivalence ratio is less than 1.2.

5. Conclusion
This research analyses the reaction path of methanol-syngas fuel and the formation and consumption of intermediate products and radicals. Sensitivity analysis of elementary reaction was carried out, and important reactions for fuel oxidation process were investigated. The effect of blending ratio and equivalence ratio on ignition delay time and flame speed was studied. It was found that the ignition delay time increased with blending ratio increasing, with the decrease of the equivalence ratio. The flame speed increases with the increase of the blending ratio. The research results can provide theoretical guidance for the application of methanol-syngas fuel in internal combustion engine.

References
[1] Sebastian Verhelst, James WG Turner, Louis Sileghem, Jeroen Vancoillie, Methanol as a fuel for internal combustion engines, Progress in Energy and Combustion Science. 70 (2019) 43-88.
[2] Bo Zhang, Changwei Ji, Shuofeng Wang, Combustion analysis and emissions characteristics of a hydrogen-blended methanol engine at various spark timings, International Journal of Hydrogen Energy. 40 (2015) 4707-4716.
[3] Changming Gong, Zhaohui Li, Lin Yi, Fenghua Liu, Experimental investigation of equivalence ratio effects on combustion and emissions characteristics of an H2/methanol dual-injection engine under different spark timings, Fuel. 262 (2020) 116463.
[4] Duc Khanh Nguyen, Sebastian Verhelst, Computational Study of the Laminar Reaction Front Properties of Diluted Methanol–Air Flames Enriched by the Fuel Reforming Product, Energy&Fuels. 31 (2017) 9991–10002.
[5] Ultan Burke, Wayne K. Metcalfe, Sinead M. Burke, K. Alexander Heufer, Philippe Dagaut, Henry J. Curran, A detailed chemical kinetic modeling, ignition delay time and jet-stirred reactor study of methanol oxidation, Combustion and Flame. 165 (2016) 125-136.