



# LAMINAR BURNING VELOCITY OF METHANOL STEAM REFORMING PRODUCTS: INFLUENCE OF CO SELECTIVITY

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## Introduction

The increasing greenhouse gas concentration in the atmosphere and dismissing of fossil fuels recent decades has heightened the need for the next generation of internal combustion engines (ICE). Using alternative fuels for ICE is one of the current directions for engine development. The simplest alcohol – methanol (CH<sub>3</sub>OH) is considered as a future fuel for spark ignition (SI) engines because of its high octane number, flame speed and heat of vaporization. The engine is able to operate under high compression ratio with a cooler intake charge. Additionally, with less heat loss, the engine efficiency further improves.

Thanks to its high H/C ratio, methanol is also acknowledged as a hydrogen carrier fuel. With low reaction temperature, methanol reforming technologies are widely employed in chemical industry to produce hydrogen rich gas. Currently, steam reforming is used most because this approach provides the highest yield of hydrogen. According to Peppley *et al.* [1], there are three overall reactions of methanol steam reforming process:



Two reactions R1 and R3 are endothermic reactions which require heat to drive the reforming. Therefore, the engine efficiency has the potential to increase with exhaust heat recovery technology for the fuel reformer. Leslie Bromberg *et al.* [2] concluded that the efficiency of methanol fuelled SI engine can be significantly improved, up to 50-60%, with the addition of hydrogen rich gas from the on-board reformer driven by engine exhaust heat. The difficulty is reforming products and their concentrations change for varying conditions, leading to the variation of laminar burning velocity and heating value. It is not difficult to calculate the heating value of reformates. However, the alteration of its burning velocity is still unknown. A study on the effect of CO selectivity on the laminar burning velocity of reformates is essential to develop the correlation for the engine simulation code.

## Numerical methodology

The mechanisms developed by Li *et al.* [3], Davis *et al.* [4] and K eromn es *et al.* [5] were examined in this

study. These three mechanisms are among the five best ones for syngas oxidation. In which, Davis's mechanism is the best one for laminar flame speed study [6]. The simulations were run using CHEM1D code. This code was developed by the Combustion Technology group, at Eindhoven University of Technology. In each case, the stationary simulation was performed with exponential differential scheme and free flame type in 200 grid points.

Assuming that the fuel conversion is 100% and the steam can be easily condensed. The product includes three gases, CO, CO<sub>2</sub> and H<sub>2</sub>. The CO selectivity is defined as the molar ratio of CO produced to the sum of CO and CO<sub>2</sub> in the product. The molar concentration of H<sub>2</sub> is calculated on the basis of molar ratio of H<sub>2</sub> to CO<sub>2</sub> and CO in R1 and R3, respectively. The mole fraction of products is shown in Table 1.

Table 1. Mole fraction of methanol reforming products

CO selectivity	CO <sub>2</sub>	CO	H <sub>2</sub>
0 %	0.25	0	0.75
20 %	0.21	0.053	0.737
40 %	0.167	0.111	0.722
60 %	0.118	0.176	0.706
80 %	0.0625	0.25	0.6875
100 %	0	0.333	0.667

The studied range of equivalence ratio was 0.6-1.2 (similar to the mixture in SI engines) and the CO selectivity was varied from 0% to 100%. All simulations were behaved in two conditions, NTP (normal temperature and pressure, 300 K and 1 bar) and engine-like condition (650 K and 20 bar). The second case, the pressure and temperature are the same as the in-cylinder pressure and temperature at ignition timing in modern SI engines with compression ratio of 10.

## Results

Figure 1 shows the laminar burning velocity of methanol reformates as a function of CO selectivity at NTP condition. Three tested mechanisms provide different data of reformate's burning velocity. Davis's mechanism gives the slowest velocity. The next is Li's mechanism and the fastest one is detected with K eromn es's mechanism. However, the simulation shows that there is almost no influence of CO selectivity-

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ty on the burning velocity of reforming products with any reaction mechanism. As showed in Fig. 2, the velocity changes less than 2% with varied CO selectivity at NTP condition. Three mechanisms demonstrate distinct trends for the effect of CO selectivity on the improvement of laminar burning velocity. The burning velocity of reformat increases with a higher CO selectivity when the Li's and Davis's mechanisms are used. The opposite trend is observed with Kéromnès's mechanism.

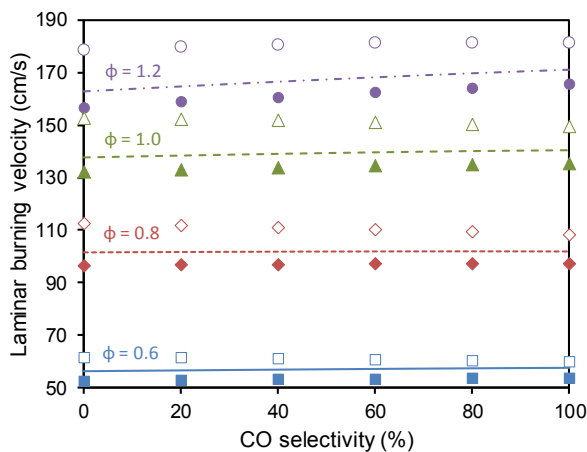


Figure 1. Influence of CO selectivity on laminar burning velocity of methanol reformates at NTP. Lines – Li's mechanism, filled symbols – Davis's mechanism, open symbols – Kéromnès's mechanism

At engine-like condition, the influence of CO selectivity becomes more significant with Li's and Davis's mechanisms. The laminar burning velocity increases to 6% and 12% with CO selectivity of 100%, respectively. Whereas, the calculation with Kéromnès's mechanism shows less impact of CO selectivity on burning velocity at this condition.

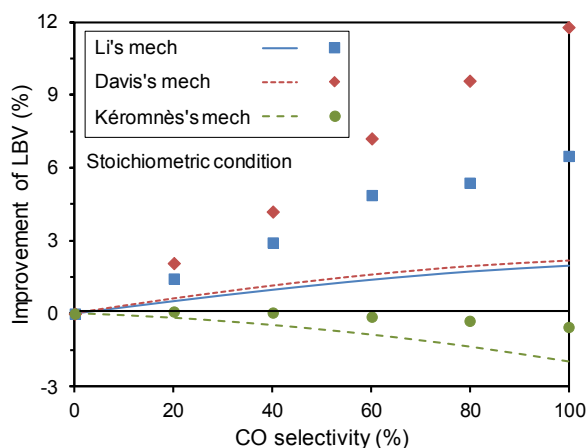


Figure 2. Influence of CO selectivity on the improvement of laminar burning velocity at NTP (lines) and engine condition (symbols) with  $\phi = 1.0$

For lean mixtures, less influence of CO selectivity is achieved with Li's and Davis's mechanisms. However, the burning velocity decreases faster with higher selectivity of CO when Kéromnès's mechanism

is used, especially at  $\phi = 0.7$  and  $\phi = 0.8$ . At rich conditions, all mechanisms show the improvement of laminar burning velocity with a higher CO selectivity.

## Conclusions

The simulations were done with three well-known syngas mechanisms at NTP and engine-like conditions. Although each mechanism shows different behaviour of laminar burning velocity changes, there is virtually no influence of CO selectivity at NTP and stoichiometric mixture. With Li's and Davis's mechanisms, CO selectivity has a greater impact at high pressure and high temperature. However, Kéromnès's mechanism presents vice versa trend.

The experimental measurement of reformat burning velocity has to be done using a constant volume combustion chamber to know the trends and validate the simulation data.

## Acknowledgements

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