

# A RAPID COMPRESSION MACHINE INVESTIGATION OF OXIDATION OF 2-METHYLTETRAHYDROFURAN AT LOW TEMPERATURE: AUTOIGNITION DELAY AND SAMPLING

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## Introduction

To reduce fuel consumption, Greenhouse Gases,  $\text{NO}_x$  and soot particles emissions, recent developments in engine technology have focused on operating engines at lower temperatures and fuel concentrations. These constraints have motivated the apparition of Exhaust Gas Recirculation (EGR) technology, and triggered interest in Low-Temperature Combustion (LTC) engines. In these conditions, combustion chemistry is more complex as it relies on the formation of peroxides. Chemical branching is degenerate and highly fuel-specific. To accommodate the use of modern fuels such as biodiesels or fuels produced from biomass, predictive models of this combustion chemistry must be constructed and validated.

Recently, the interest has grown on the use of liquid fuels produced from lignocellulosic biomass. Among those, 2-methyltetrahydrofuran (2-MTHF) has numerous advantages in terms of ease of production [1] and compatibility with existing fuels derived from fossil resources [2]. Moshammer et al. studied this fuel at high temperatures in flames and released a kinetic detailed mechanism [3]. Simmie provided key rate constants for the oxidation of 2-MTHF relevant for high temperature kinetics [4].

To our knowledge, there are no data on the oxidation of 2-MTHF in the low temperature combustion temperature range. Thus, an experimental study was performed at PC2A, in engine-relevant conditions to provide an understanding of the reaction pathways involved in its oxidation. This study complements the investigations on lignocellulosic biofuels, started with the study of tetrahydrofuran (THF).

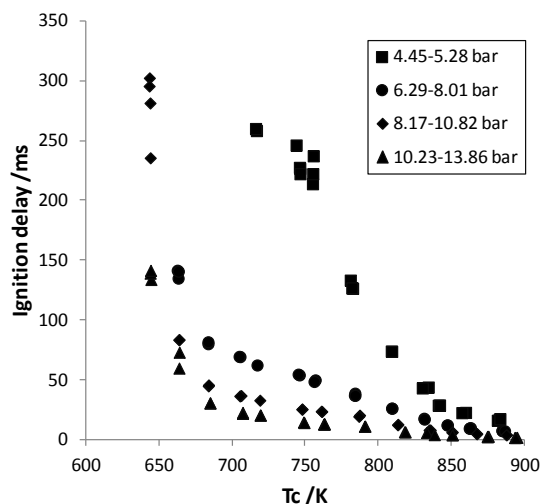
## Experimental

Rapid Compression Machine (RCM) studies provide a well controlled environment for such experimental studies, for pressures from 5 to 30 bar and temperatures from 600 to 1000 K relevant to these engine conditions. They are therefore suited to provide ignition delay data that constitute global model validation data.

The RCM at University of Lille also provides the opportunity to extract samples of the reacting mixture during the ignition delay, providing insight into the composition of the unburned hydrocarbons formed in the cool flame, the main reaction pathways, but also detailed model validation data.

## Results and discussion

Ignition delays were measured for top-dead center pressures between 3.5 and 21 bar and  $T_c = 650$ – $900\text{K}$ , as well as cool flame delays, when detected. Some results are presented in figure 1. When plotted against temperature, ignition delays exhibit a non-Arrhenius behavior. A plateau is visible, showing a low-temperature reactivity of 2-MTHF, but not leading to a negative coefficient of temperature, usually happening for alkanes between 700 and 850K.



**Figure 1: Ignition delay times of stoichiometric 2-MTHF/air mixtures at different pressures and temperatures.**

Ignition delays of 2-MTHF were compared to those of tetrahydrofuran (THF), measured in the same RCM [5]. In the same conditions, 2-MTHF is slightly less reactive than THF.

Sampling of the reacting mixture 2-MTHF/air was performed for different times during the cool flame, in order to identify and quantify the stable intermediates produced in the low temperature range.

Among intermediates identified in the cool flame region, the most abundant are, for example, dimethylfurans, dihydromethylfurans, 1-propen-2-ol acetate, methyl-dihydrofuranones. A total of 27 have been identified and quantified along the ignition delay, providing detailed kinetic model validation data.

## Conclusions

An experimental study of the oxidation of 2-methyltetrahydrofuran was performed in a rapid compression machine, in engine-relevant conditions ( $\phi = 1$ ,  $T_c = 650\text{-}900\text{ K}$  and  $P_{tdc} = 3.5\text{-}21\text{ bar}$ ). Cool flame and ignition delays were measured. The evolution of ignition delays with temperature exhibits non-arrhenius behavior, forming a plateau. Compared to THF, 2-MTHF is slightly less reactive.

Stable intermediates of the oxidation of 2-MTHF were identified from sampling of the reacting mixture in the RCM during the cool flame. The concentration profiles of 27 species during a two-stage ignition delay were measured.

Both of those experimental data sets can help to build and validate a kinetic detailed mechanism of the oxidation of 2-MTHF at low-temperatures.

## Acknowledgements

The post-doctoral researches of Y. Fenard are funded by Total.

## References

- [1] Illés, Á., Farkas, M., Gombos, E., Zügner, G. L., Novodárszki, Gy., Dóbe, S., Proceedings of the European Combustion Meeting (2015)
- [2] García, A., Monsalve-Serrano, J., Heuser, B., Jakob, M., Kremer, F. and Pischinger, S., Energy Conversion and Management, 108, 243:254 (2016)
- [3] Moshhammer, K., Vranckx, S., Chakravarty, H. K., Parabb, P., Fernandes, R. X. and Kohse-Höinghaus, K., Combustion and Flames, 160(12), 2729:2743 (2013)
- [4] Simmie, J. M., Journal of Physical Chemistry A, 116, 4528:4538 (2012)
- [5] Vanhove, G., Yu, Y., Boumehdi, M. A., Frottier, O., Herbinet, O., Glaude, P.-A., and Battin-Leclerc, F., Energy Fuels, 29 (9), 6118:6125 (2015)