A rapid compression machine kinetic study of the effect of hydrogen on the ignition delay times of *n*-pentane, 3-pentanone & 1-pentene in the low temperature combustion regime

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Atmospheric concentrations of greenhouse gases (GHGs) are rising with the increase in transportation vehicles and their daily use. To be able to contain this problem, alternative fuels must be found; they must be as friendly as possible to our environment. Hydrogen, being a carbon free gas, is an excellent example of a fuel that does not participate in producing carbon dioxide and methane; two important GHGs [1,2]. But using it alone as a fuel is not recommended according to its hazard [3,4]. A solution consists in blending hydrogen with other fuels to enhance the efficiency of the engine [1] and decrease the pollutant emissions into the atmosphere. In order to integrate this blend into the existing combustion systems, and well understand its behavior, it is mandatory to understand the kinetics of combustion of fuel and biofuel representatives with hydrogen at high and low temperatures. There is a lack in the literature on the influence of hydrogen on the combustion of fuels in the low temperature range of combustion. We propose to investigate the reactivity of fuel/hydrogen/'air' mixtures via ignition delay times measurements inside the ULille rapid compression machine. This work is complemented by detailed kinetic modeling allowing a deeper understanding into the interactions between hydrogen and different fuel molecular structures on ignition delay times in the low temperature region (<1000K).

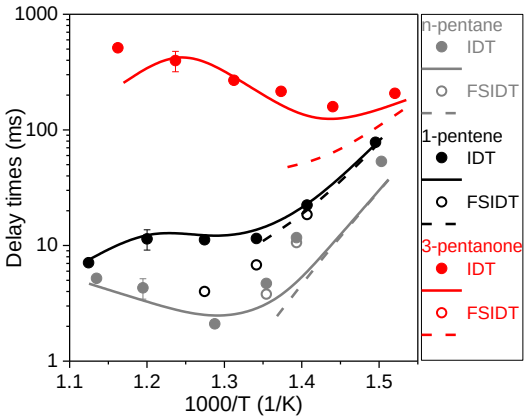

Fig. 1- Experimental (symbols) and simulated (lines) first stage of ignition (FSIDT) and total ignition (IDT) delay times of stoichiometric 50%fuel/50%H_2 / 'air' at 1.5 MPa.

In this study, C_5 chain molecules - *n*-pentane, 3-pentanone, and 1-pentene - have been chosen to blend with hydrogen. This choice helps in understanding the different effects of the chemical function of each

fuel. Kinetic models from the literature [5–7] are used to analyze the balance between chain branching, propagating, and terminating channels after assessing their performance in the simulation of our experiments as shown in Fig. 1. In broad context, three main categories are responsible for the ignition properties: (i) initiation reactions that generate a distribution of organic radicals, $\dot{R}$; (ii) competing unimolecular decomposition of $\dot{R}$ and bimolecular reaction of $\dot{R}$ with O_2; (iii) decomposition mechanisms of peroxy radical adducts $R\dot{O}_2$, including isomerization via $R\dot{O}_2 \rightleftharpoons \dot{Q}OOH$.

Ignition delay times are measured in different pressure conditions (p = 10, 15, 20 bar) and at different equivalence ratios (0.5 and 1). Each fuel was studied with different proportions of hydrogen (0%, 25% and 50%). *n*-pentane and 3-pentanone show a minor increase in ignition delay times with the increase of hydrogen percentages. However, there is no significant effect of the increase of hydrogen on 1-pentene. This effect is explained by performing sensitivity analyses.

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