On the influence of hydrogen on the low-temperature combustion kinetics of biofuels

Organization/Company: PC2A

Research field: Chemistry/Analytical chemistry and Physical chemistry

Researcher profile: First Stage Researcher

Application deadline: 30/04/2021

Location: France/Villeneuve d'Ascq

Type of contract: Temporary

Job status: Full-time

Hours per week: 35

Offer starting date: 0110/2021

Keywords:

Biofuels, hydrogen, combustion, ignition delay times, reactivity, rapid compression machine, pollutants, sampling techniques, gas phase chromatography, mass spectrometry, kinetic modeling.

Offer description:

Kinetic mechanisms of low temperature oxidation of biofuels with hydrogen. Experimental study through measurement of ignition delay times in a rapid compression machine and time-resolved analysis of the reactive mixture, and kinetic modeling.

Even as the global market share of battery electric vehicles increases, the environmental costs of manufacturing, running and disposing them, the lack of recharging infrastructure, and the limited ranges for heavy vehicles, the opportunity to use internal combustion engines (ICEs) fueled with renewable hydrogen has attracted attention in the past years. Strategic plans to decrease primary energy use, introduce low-carbon fuels and facilitate modal shifts. Taking a prominent place in these strategic plans is hydrogen as an energy carrier. A number of manufacturers are now leasing demonstration vehicles to consumers using hydrogen-fueled internal combustion engines (H2ICEs). This dual-fuel application shows a decrease of NO_x, smoke, CO and unburnt hydrocarbons emissions, both for H_2-diesel/biodiesel and H_2-gasoline/ethanol.

However, fundamental studies on the impact of hydrogen on the low temperature combustion kinetics of fuels are scarce, especially with oxygenated fuels produced from biomass. The kinetics in the low temperature combustion range are initiated by the interaction of primary radicals from fuels and molecular oxygen, leading to an increase of the reactivity in the temperature range 650-800 K. They affect internal combustion engines operation and ultimately efficiency and pollutant emissions.

A global parameter is widely used for the characterization of a fuel: the ignition delay time. It describes the time required for a fuel / air mixture to ignite under known conditions of temperature and pressure. Studying the ignition delay time allows the refinement of the fuel composition and fuel / air equivalence ratio required for an optimal performance of an engine. In addition, experimentally measured ignition delay times are used as validation targets for detailed predictive kinetic models. Such detailed kinetic models are then used to better understand the kinetics influencing combustion. For more information, please visit pc2a.univ-lille.fr.

During this PhD, we propose to extend the measurement of the ignition delay times of different fuels by mixing them with H_2 , in order to assess the dependence on the chemical nature of the fuel – alkane, alkene, alcohol or ketone – and cover the potential chemicals that could be found in fossil fuels or biofuels. The facility used at PC2A is a rapid compression machine, which allows, on top of measuring ignition delays, to sample and quantifiy intermediates formed during this ignition delay. The analysis of results will make it possible to draw a trend in the interaction of chemical functions with H_2, and build predictive kinetic models of the observed reactivity.

The objectives of the thesis are to:

• Understand and deepen the knowledge of the auto-ignition mechanisms of fuels and biofuels in the presence of hydrogen in the low temperature ranges of combustion, through experimental and modeling work,

• Evaluate the need for, and perform theoretical calculations in order to strengthen the description of the combustion of fuels / biofuel with hydrogen,

• Propose recommendations on fuel mixtures allowing cleaner and more efficient combustion in internal combustion engines.

Offer requirements:

Required education level: Master Degree in chemistry or equivalent

Experience in analytical chemistry, kinetic modeling, ab initio calculation or combustion will be appreciated.

To apply:

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