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EXPERIMENTAL STUDY OF RICH ETHYL VALERATE FLAME AT LOW PRESSURE

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Abstract

Biomass is considered as an important source for the production of liquid fuels. Among them, ethyl valerate can be produced from lignocellulosic biomass. Indeed, levulinic acid obtained from lignocellulose can be converted into esters (valerate radical) by hydrogenation and esterification. Few results are available to characterize the combustion of these esters at high pressure and none at low pressure. In this work, we study of ethyl valerate at low pressure (55 mbar) in a Spalding-Botha burner in order to characterize its combustion kinetics. The main challenge is to upgrade the test bench, combining an evaporation system for the ethyl valerate, the combustion chamber, a compression system, and a gas chromatography. The rich flame of ethyl valerate shows the presence of oxygenated compounds as first intermediate species of its combustion. The species measured will allow the construction of a detailed kinetic model of ethyl valerate combustion at low pressure.

Introduction

The increasing demand of energy, the decreasing availability of fossil fuels, and the climate changes are important challenges of this century. To alleviate these issues, the diversification of the energy mix is proposed including a major contribution from biomass, also in the form of biofuels [1-4]. Among them, valerate esters can be produced from lignocellulosic biomass. Indeed, levulinic acid obtained from lignocellulose can be converted into esters (valerate radical) by hydrogenation and esterification. From these esters, methyl and ethyl valerate ($C_6H_{12}O_2$ and $C_7H_{14}O_2$) can be used in spark ignition engines. Heaviest ones, propyl and butyl valerate ($C_8H_{16}O_2$ and $C_9H_{18}O_2$) can be used in diesel engines [3-6]. The present study is focused on ethyl valerate.

Recently, Dayma et al. [7] studied experimentally the ethyl valerate combustion at high pressure (10 atm) in a jet stirred reactor, and the laminar burning velocities in a spherical combustion chamber. According to the experimental results, they elaborated a mechanism containing 524 chemical species and 2431 reactions. However, the validation of such mechanism at low pressure has not yet been performed. This study thus focused on the experimental structure of a rich premixed flat flame of ethyl valerate/ O_2 /Ar at low pressure. The flame has been stabilized on a Spalding-Botha type burner at low pressure, 55 mbar, to accurately measure the profiles of species produced and consumed during the combustion. The chemical compounds have been detected and identified by gas chromatography. Working with esters however required some modifications of the experimental setup. We had to adapt an evaporation system for the ester, so that it can be fed into the combustion chamber in gaseous phase.

Approach

The experimental set up is composed by an evaporation system (EV), the combustion chamber (CC), a compression system (CS) and the gas chromatography (GC). The ethyl valerate has a boiling point of 145°C at atmospheric pressure. To have it in a gaseous phase, a evaporation system has to be designed. We use a system containing two mass flow meter controllers and a controlled evaporator.

The combustion chamber where the flat flame of ethyl valerate is stabilized at 55 mbar, is a movable Spalding-Botha-type burner of 8 cm in diameter. A conical quartz nozzle is facing the surface of the burner with an angle of 45° within 2 cm and 0.2 mm of a small hole that allows sampling to be performed through the flame. To keep the sample at high temperature and to avoid condensation in the pipes, a heated ribbon at 200°C is used after the nozzle.

As the experiment is performed at low pressure and the GC is working at atmospheric pressure, a compression system is needed to increase the pressure of the collected gas before injection. The pressure after the CC is 20 mbar. The sample is at 1700 mbar after the compression system. The compression is nearly isothermal as the mass of gas is low. The temperature of the gas is around 72°C as the compression cylinder is also heated up to avoid condensation during compression.

The gas chromatography allows analyzing only stable chemical compounds. However, different isomers can be also separated and analyzed with this method. The GC (TOGA) is used to analyze fresh to burned gas and has three columns (CP SIL CB5 for the hydrocarbon and oxygenated compounds and Molsieve in series with RTX1 for the permanent gases). Two detectors (TCD and FID) are used to measure concentrations of species. This GC has a methanizer, that allows converting carbon monoxide (CO), carbon dioxide (CO₂) and formaldehyde (CH₂O) into methane (CH₄). The RTX1 column is used only for the flow rate restriction before the analysis of separated compounds from CP SIL CB5 and Molsieve columns.

Results and discussion

The first step is the stabilization of the flame in the experimental conditions at low pressure. The composition of the rich ethyl valerate flame is thus : 4.6 % Ethyl valerate – 32.3 % Oxygen – 63.1 % Ar, with an equivalence ratio of 1.3. The total flow rate is 6.14 l/min and the ratio C/O is 0.43. In these conditions there is no soot formation during combustion.

In this paragraph, we present only the FID results in which the integration of the pic area for each species studied is related to the distance of the burner in millimeter (mm). The integration pic area is measured from the FID signal that is in picoAmpere (pA).

The next figures present the intensity profiles of species detected by gas chromatography. In figure 1, the profile of ethyl valerate shows that the flame front is at 4 mm. The reaction zone is between 2 and 8 mm for all the species detected by the GC. As shown in figures 4, 6, 7, 8 and 9, methanol, acetic acid, formic acid, acetone, and valeric acid respectively, appear before ethanol (figure 5) and formaldehyde (figure 2) and have their maximum concentration at 4 mm. This distance is equivalent with the lowest concentration of ethyl valerate as shown in figure 1. As the ethyl valerate is an oxygenated compound, we remark that the behavior of its combustion is to form in its consumption the oxygenated compounds before the hydrocarbons. The hydrocarbons as methane (figure 11) and propane (figure 3) are formed later in the flame and have their maximum concentration at 8 mm.

To build a kinetic model, mole fractions of different species are needed. The calibration is ongoing in order to convert all intergration areas into mole fractions.

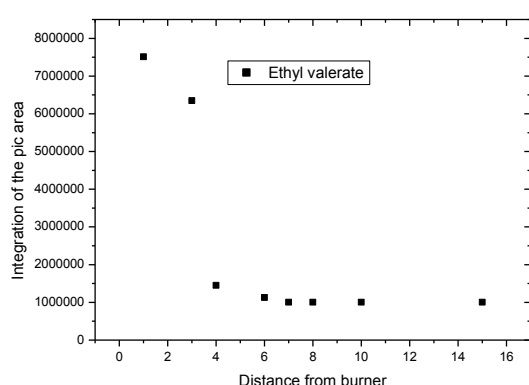


Figure 1

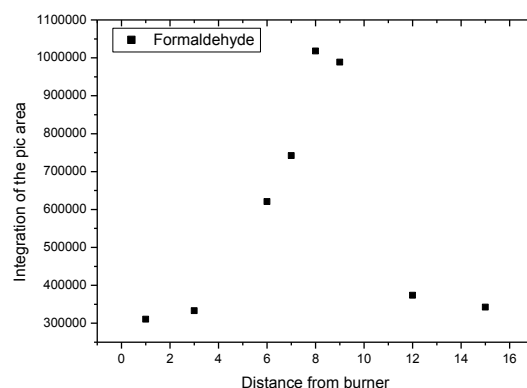


Figure 2

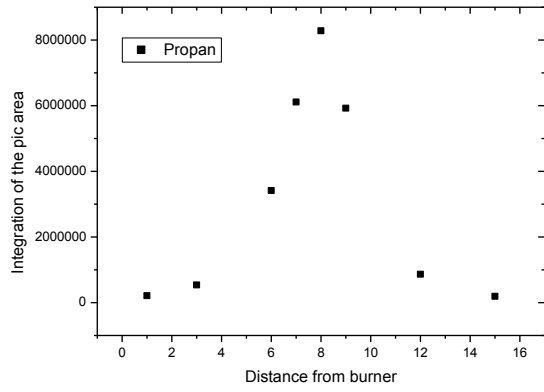


Figure 3

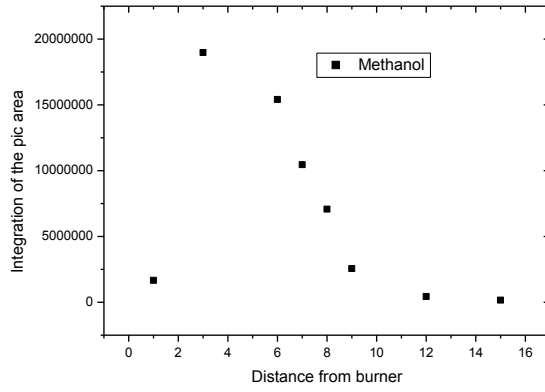


Figure 4

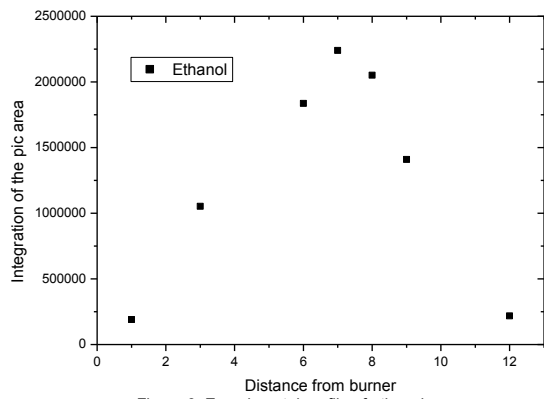


Figure 5

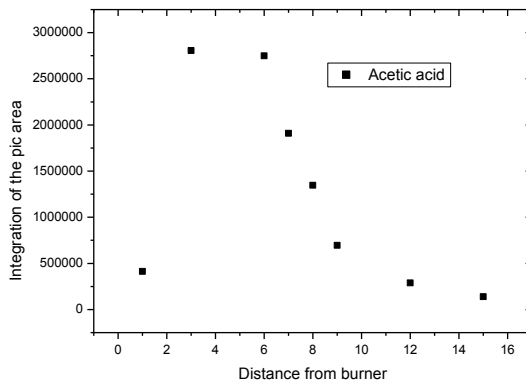


Figure 6

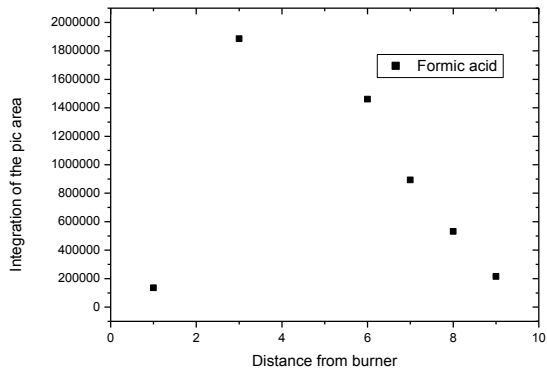


Figure 7

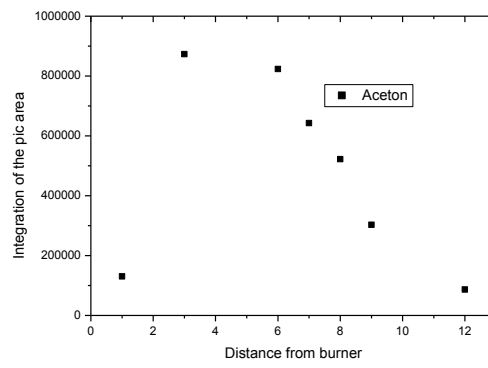


Figure 8

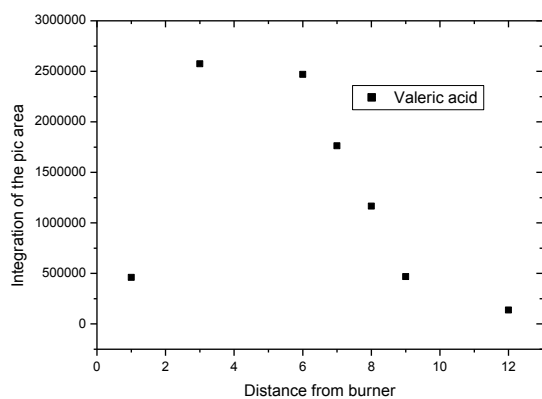


Figure 9

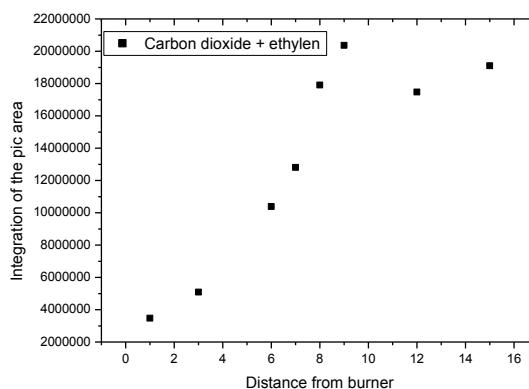


Figure 10

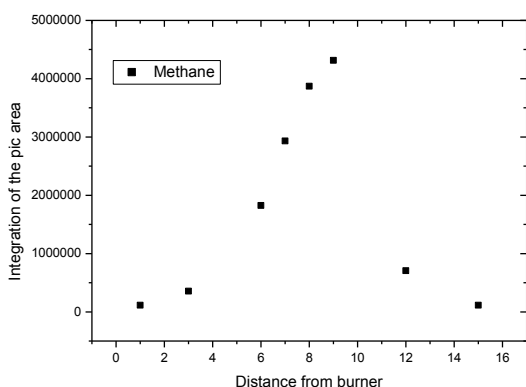


Figure 11

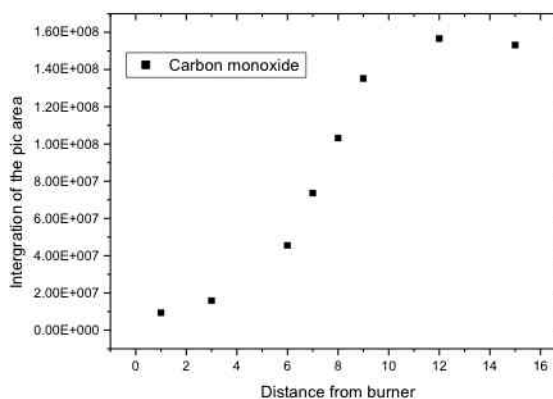


Figure 12

Perspective

The next step is the validation of Dayma mechanism at low pressure. It is envisioned that the kinetic model elaborated by Dayma et al. [7] will complete the "UCL" mechanism [9-10] already validated against several hydrocarbons and oxygenated species flames. Moreover, it will be valorize in other combustion modeling efforts. In particular, the mechanism will be coupled to Computational Fluid Dynamics (CFD) tools in order to study the performance of these esters in Homogeneous Charge Compression Ignition (HCCI) engines.

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