Kinetic modeling of ethyl pentanoate combustion in laminar premixed flames

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Introduction

Biofuels can be part of the future energy matrix as an easily storable and readily usable energy carrier. However the sustainability of the current biofuels is doubted, therefore other possible biofuels from waste biomass streams gain interest, like pentanoate esters. They can be produced from acid hydrolysis of lignocellulosic materials and their properties are similar to gasoline or diesel, depending of the length of the alcohol group [1].

The behavior of mixtures of pentanoate esters and fossil fuel is already investigated for different types of engines. A comparison of a 20 vol% butyl and pentyl pentanoate mixed with diesel and pure diesel as reference, showed no significant modification in the emissions and performances [2]. The same conclusion was found when pure methyl and ethyl pentanoate esters were compared with gasoline [3]. Lange et al. tested a blend of 15 vol% ethyl pentanoate in regular gasoline engine and found no measurable impact on engine wear, oil degradation, deposits and emissions. They concluded that the good octane properties of ethyl pentanoate benefits the power generation [1].

However, the combustion kinetics of these potential biofuels should be determined, allowing making realistic simulations of the performance of pentanoate esters in vehicle engines. We investigated the combustion of one species of pentanoate esters, ethyl pentanoate, in a premixed flat laminar flame at low pressure. The data provided by these measurements is used to determine the kinetic parameters of ethyl pentanoate combustion using OpenSmoke software.

Experimental set-up

The experimental set-up to take samples consists of an evaporation system, a flat flame burner and a gas chromatography (GC) column connected with a flame ionization detector (FID) and a thermal conductivity detector (TCD) (Figure 1).

Four gas bottles (argon, oxygen, ethylene and hydrogen) deliver the necessary input to ignite the burner and to obtain different equivalence ratios for diluted mixtures at low pressure. The fuel, in this case ethyl pentanoate, is kept at liquid state in a pressurized vessel and is mixed with argon at a heated evaporator. Other liquid fuels can also be vaporized by this system. The mixture of fuel and argon is led to the combustion chamber through a heated ribbon to minimize the condensation of ethyl pentanoate and at the inlet of the combustion chamber it is mixed with the other gasses. The burner operates at low pressure around 55 mbar. The main advantage of a flat laminar burner is that the distance from the burner is correlated to the reaction propagation, meaning that further away from the burner more final reaction products will be measured. When moving the burner, a sample is taken through a quartz cone at different positions in the flame. The sample is analyzed by the GC-TCD and FID. After calibration the derived results can be converted to mole fractions.

In this way, the mole fractions of present reactants at different distances in the flame can be measured and mole fraction profiles can be deduced. The mole fraction profiles can then be used to validate a kinetic model.

Since the concentrations of the sample are near the detection limit of the two detectors, a piston injection system (not on Figure 1) to increase the concentration was installed between the burner and the GC.

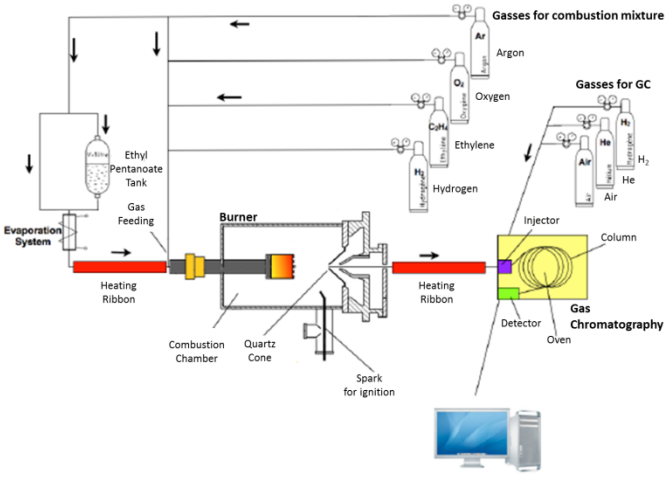

Figure 1: Experimental setup consists of three main parts: the evaporation system, the flat flame burner and the detection devices

Kinetic modeling

The mole fraction profiles obtained for the reactants and the reaction products by the experiments throughout the flame and a mechanism established by Dayma et al. [4] are used to derive the detailed kinetic model for ethyl pentanoate combustion. The measurements were done for three different flames: a lean, a stoichiometric and a rich one, with equivalence ratios of 0.79, 1.08 and 1.35 respectively. So the influence of the equivalence ratio on the kinetic behavior can be established.

The OpenSMOKE framework [5], developed at Politecnico di Milano, is used to simulate the combustion of ethyl pentanoate with the measured mole profiles and mechanism as input. The GC-TCD/FID is only capable to detect vaporized non-decomposed intermediates and reactants. The behavior of the radicals and ions is estimated by already available kinetic data.

Results

The measured intensity profile for some species in function of the distance from the burner, and thus also the reaction propagation, are shown in Figure 2 and 3. The fuel is consumed in the flame as seen in Figure 2. In Figure 3 we see that that CO_2 and CO are formed as reaction products and that HCOH, aceton, ethanol and methane are some of the formed intermediates.

Acknowledgments

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OpenSMOKE: numerical modeling of reacting systems with detailed kinetic mechanisms

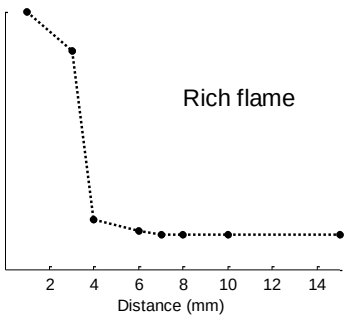

Figure 3: The measured signal for ethyl pentanoate with FID decrease in function the distance to the burner

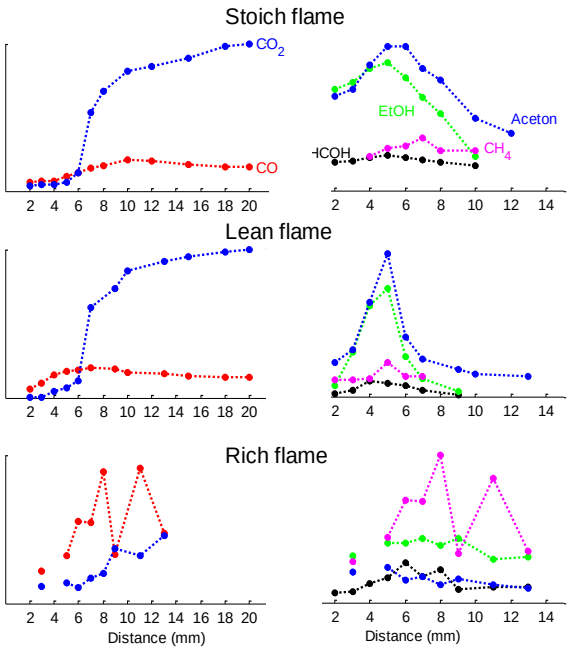

Figure 2: The measured signal profiles for the reaction products CO_2 and CO and for some of the measured intermediates for the three different flames