EXPERIMENTAL AND KINETIC MODELING OF A RICH METHYL PENTANOATE FLAME AT LOW PRESSURE

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Introduction

Pentanoate esters are seen as a new class of biofuels, which can be produced from lignocellulosic biomass. Commonly the conversion of lignocellulosic material to biofuels needs advanced and complex processes. However, pentanoate esters can be produced more easily with levulinic acid as intermediate [1-3]. The full process is already commercialized under the name Biofine [4].

Pure pentanoate esters and mixtures of pentanoate esters with conventional fuel are already tested in engines [1, 5-7]. Some authors report no significant difference, while others found more NOx and small particles in the pentanoate esters exhaust.

Besides the engine tests, kinetic models for the combustion of pentanoic esters are collaborated [8-9].

In this abstract, the experimental work on a rich methyl pentanoate flame is presented. The results are used to elaborate and validate a kinetic model for the combustion of methyl pentanoate at low pressure. Currently, experimental work on a stoichiometric flame is processed; however no results of the stoichiometric flame will be discussed.

Experimental set-up

The experimental set-up consists of three main parts: an evaporation system for the fuel, a Botha-Spalding burner and gas chromatography equipment. The fuel is evaporated and mixed with oxygen and argon to obtain premixed and diluted conditions in the combustion chamber.

The combustion chamber consists of a circular burner with a diameter of 8 cm. The pressure in the combustion chamber is kept constant during the experiments at 55 mbar. Sampling is carried out with a quartz cone, opposite placed from the burner. The diameter of the cone is 0.2 mm. The distance between the burner surface and the sampling cone can be adjusted manually by moving the burner. By this way, samples at difference distances, related to different times in the combustion process, can be taken.

Gas chromatography followed by two detectors: a thermal conductivity detector (TCD) and flame ionization detector (FID), is used to analyze the samples. The sample is compressed and expanded to 1 atm prior injection in the GC to obtain detectable concentrations.

The temperature of the rich flame is measured using a PtRh6%-PtRh30% thermocouple coated with a ceramic layer of $BeO-Y_2O_3$ and a diameter of 0.1 mm. The radiation losses during the measurements are accounted by the electrical compensation method. The temperature profile of the stoichiometric flame is not measured yet.

Experimental and simulations results

Sixteen species are identified and quantified, namely the fuel methyl pentanoate (MPE), formaldehyde (CH_2O), acetaldehyde (CH_3CHO), propane (C_3H_8), ethanol (C_2H_5OH), acetone (CH_3COCH_3), formic acid (HCOOH), acetic acid (CH_3COOH), CO_2, CO, methane (CH_4), ethylene (C_2H_4), acetylene (C_2H_2), hydrogen, oxygen and argon. To convert the areas obtained by GC-TCD/FID to mole fraction, a response factor was acquired by calibration for the different species.

Two flames with different equivalence ratios are investigated (Table 1). Only the rich flame will be further discussed.

The mechanism used for the simulations of the MPE combustion is composed out of two other mechanisms. The main mechanism for the C_1-C_4 species is the UCL mechanism validated for low pressure [10], where the mechanism for MPE oxidation from Dayma is added [11]. The obtained mechanism consists of 1668 reactions for 269 species. Simulations for the rich flame where conducted with the OpenSMOKE software [12].

For the rich flame the experimental results fit the simulation results for MPE, CO_2 and H_2 (Figure 1). For CO a higher concentration is found experimentally than in the simulations.

Table 1: Composition of the discussed rich flame and the stoichiometric flame which is still in progress

| φ [-]	MPE (mole%)	AR (mole%)	O_2 (mole%)
1.41	4.4	70.8	24.8
1.15	4.1	67.1	28.8

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The post combustion zone mole fraction of the water is calculated from the measured temperature and the mole fractions for CO, CO_2 and H_2 in the burned gasses.

For some of the intermediates, such as CH_4, the experimental result and simulations are of the same order of magnitude. For other intermediates, such as C_2H_4 and CH_2O, the simulated mole fraction profiles underestimates or overestimates the experimental one, respectively. The kinetic model has to be improved to predict perfectly these experimental values.
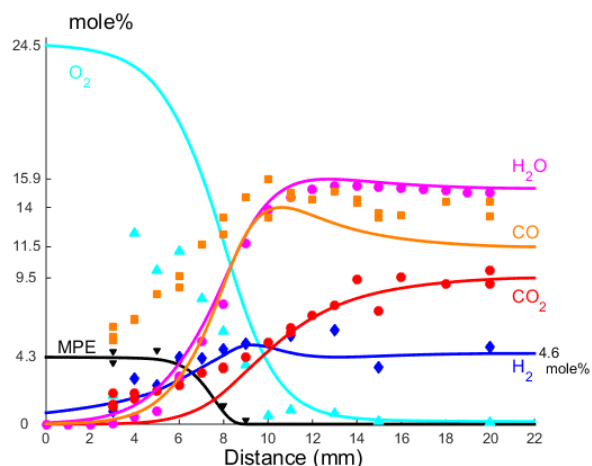
Figure 1: Experimental (symbols) and simulated (lines) mole fraction profiles of MPE, H_2, O_2, CO, CO_2 and H_2O in the rich MPE flame.
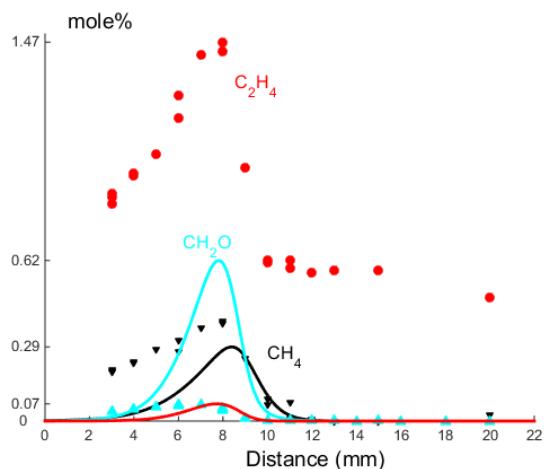
Figure 2: Experimental (symbols) and simulated (lines) mole fraction profiles of CH_2O, CH_4 and C_2H_4 for a rich MPE flame.

Conclusions

The experimental results for the combustion of a rich MPE flame at low pressure matches the simulations. For MPE, H_2O, CO_2 and H_2 a good match is found. However improvement is needed for most of the intermediate species.

For the stoichiometric flame the temperature profile needs to be measured and then an improved kinetic model for the combustion of MPE will be elaborated and validated for different equivalence ratios.

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