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EXPERIMENTAL AND NUMERICAL STUDY OF STRUCTURE OF A PREMIXED FLAME OF METHYL DECANOATE

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Abstract

The structure of premixed methyl decanoate/oxygen/argon flames stabilized on a flat burner at atmospheric pressure was studied by the molecular-beam mass spectrometry (MBMS). Experimental results were compared with the results of the computer modeling. The computer modeling has been performed by two different chemical kinetics mechanisms proposed in literature. The main products of methyl decanoate combustion were identified by MBMS technique. Analysis of the initial stages of methyl decanoate decomposition showed that free radical reactions play significant role in methyl decanoate oxidation.

Introduction

The increase of energy consumption in the world motivates the search of new renewable kinds of fuels. To avoid the need of the development and creation of new kinds of engines, most attention is given to compounds similar in physical properties to the components of traditional fuels derived from petroleum. Biodiesel fuels based on methyl esters derived from vegetable oils conform well with the latter condition. The detailed knowledge of the combustion kinetics of methyl esters will determine optimum composition of biodiesel or its blends with traditional diesel fuel for the use in various fields.

At the moment, the greatest number of studies were focused on the oxidation kinetics of methyl decanoate. This ester is significantly lighter than real main components of biodiesel, which greatly facilitates working with it, but at the same time it has sufficiently long alkyl chain, so that information about its oxidation can be effectively used for developing the mechanisms of biofuels combustion. Oxidation of methyl decanoate was previously investigated experimentally, but there is a lack of experimental data on pre-mixed flames. These data are necessary to validate the numerical oxidation mechanisms in the flame conditions. In this regard, the aim of this work is to acquire new experimental data on the thermal and chemical structure of a premixed methyl decanoate flame at atmospheric pressure and to validate the detailed mechanisms of its combustion available in the literature.

Approach

Premixed stoichiometric ($\varphi=1.0$) methyl decanoate ($C_{11}H_{22}O_2$, MD) flame stabilized on the Botha – Spalding burner at the atmospheric pressure has been studied. The initial fuel mixture had the following composition (in mole fractions): MD/O₂/Ar = 0.01/0.157/0.833. Linear flow rate of the fresh mixture at the burner exit was $v_0 = 14.9$ cm/s under standard conditions (1 bar, 25 °C). The mole fraction profiles of the various compounds in the flame were derived by the MBMS method with soft electron impact ioniza-



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tion. Sampling is performed by a thin-walled (80 micron) quartz probe with the opening angle of 40° and the orifice at the tip 80 microns in diameter.

An independent analysis of the intermediate products of combustion was also performed using a quartz probe connected to a glass bottle. Before the experiment, the bottle was evacuated with a vacuum pump to a pressure of about 1 Torr, then the pump was shut off using a valve and the sampling was performed. Subsequently, the sample in the bottle was diluted with argon and analyzed using gas chromatography-mass spectrometer (Agilent

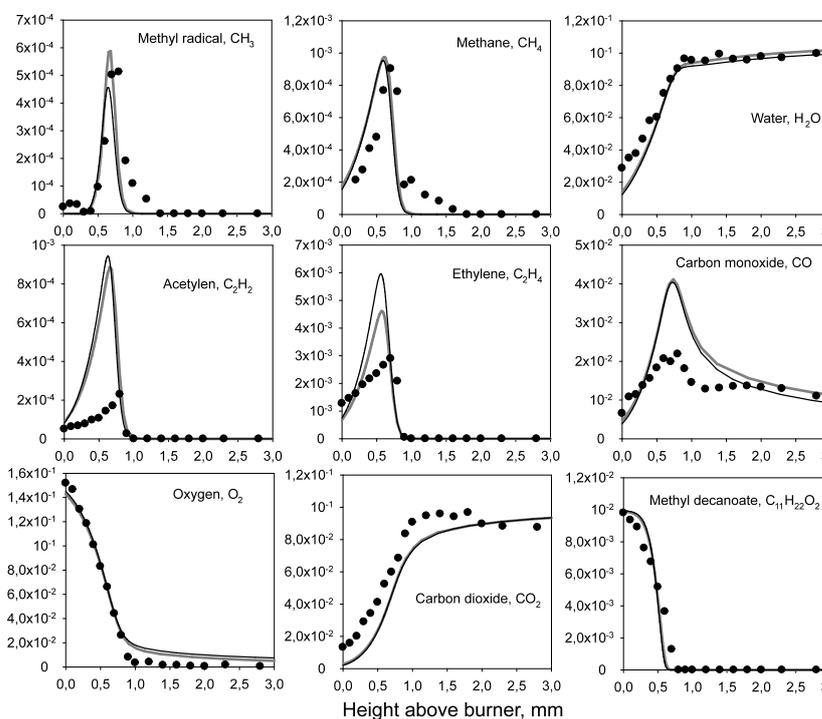


Figure 1. Mole fraction profiles of flame species. Symbols: experiment; curves: modeling.

HP6890/5973N).

The temperature profile in the flame was measured by the Pt/Pt+10%Rh thermocouple (the thickness of the junction was about 0.02 mm) with anticatalytic coating.

The structure of the flame has been modeled by the PREMIX program from the CHEMKIN II package. To model the structure of the flame 2 versions of the combustion mechanism of the methyl decanoate were used. The first mechanism is taken from [1] and contains 649 compounds and 2998 reactions. The second mechanism is a reduced mechanism proposed in [2]. It involves 530 species and 2396 reactions.

Results and discussion

Figure 1 shows measured and calculated (using two abovementioned mechanisms) mole fraction profiles of various species identified in the flame. As can be seen, both mechanisms reproduce well the experimental results for the main stable products (CO, CO₂, H₂O), reagents (MD, O₂) and a number of intermediates, however there are some differences. The most significant differences between the experimental data and simulation results are observed for carbon monoxide, acetylene and ethylene. This can be due to insufficient accuracy of the kinetic parameters of reactions involved in the mechanisms.

Gas chromatography-mass spectrometric analysis of the products of the methyl decanoate combustion indicates that the decomposition of the

original fuel proceeds for various bonds within the molecule with very little impact on their energy decomposition process. This process is typical for reactions involving free radicals.

We can assume that such methyl decanoate combustion reactions predominate over unimolecular decay. Based on the comparison of the measurement results of mole fraction profiles of different stable species and intermediates with the simulation results for two different mechanisms of transformation of methyl decanoate in the flame, we can conclude that the mechanisms used reproduce adequately the structure of the flame, as well as satisfactorily predict the possibility of formation of various intermediates upon the conversion of the methyl decanoate in the reaction zone.

Conclusions

In this work we present new experimental data on the structure of laminar premixed flame of methyl decanoate, acquired by the methods of MBMS and gas chromatography-mass spectrometry. Numerical modeling of the structure of the flame using two different detailed mechanisms of chemical reactions was performed. The main primary stages of the methyl decanoate decomposition are analyzed. Comparison of the results of the experiment and the simulation showed in general a good agreement between them, and also confirmed the consistency of methyl decanoate decomposition schemes used in the mechanisms.

Acknowledgements

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References

- [1] **Sarathy S.M., Thomson M.J., Pitz W.J., Lu T.** An experimental and kinetic modeling study of methyl decanoate combustion // Proc. Combust. Inst. – 2011. – V. 33. – P. 399-405.
- [2] **Diévert P., Won S. H., Dooley S., Dryer F. L., Ju Y.** A kinetic model for methyl decanoate combustion // Combust. Flame. – 2012. – V. 159, № 5. – P. 1793-1805.