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**Berlin Institute of Technology
(TU Berlin)**

Prof. Dr. Frank Behrendt
Fakultät III: Prozesswissenschaften,
Institut für Energietechnik

Chair Energy Process Engineering and
Conversion Technologies for
Renewable Energies (EVUR)
Fasanenstr. 89
10623 Berlin

Contact
info@flame-structure-2014.com
frank.behrendt@tu-berlin.de

Berlin Institute of Technology • Fasanenstr. 89 • 10623 Berlin

King Abdullah University of Science
and Technology

Hatem Selim

KAUST

Thuwal, Saudi Arabia

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Confirmation of paper submission

Name: Hatem Selim
Email: hatem.selim@kaust.edu.sa
Co-author: Arnas Lucassen
2nd co-author: Nils Hansen
3rd co-author: Mani Sarathy
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Abstract

Improving the knowledge on hydrocarbon fuels combustion will lead to combustion efficiency enhancement along with emissions control. Low-pressure combustion of premixed flat flame of isomeric fuels (2- and 3-methyl heptane) was investigated using vacuum UV synchrotron radiation for species ionization. Major species, intermediate species, radicals, and isomers were quantified using a time of flight mass spectrometer. Photoionization efficiency was used to differentiate between isomers. The location of the methyl group on the heptane hydrocarbon chain proved to have a pivotal role on the intermediate species and isomers. However, the effect proved to be minimal for the major end products such as CO, CO₂ and H₂O. Numerical simulations were conducted for comparisons with the experimental results. The trends were captured successfully for all species, yet with some qualitative discrepancies for the intermediate species.

Introduction

The stringent environmental regulations and the shrinkage of fossil fuels reserves raised a problematic challenge in all combustion applications. This challenge requires development of more efficient, yet less pollutant, transformation of the fuels chemical energy into thermal energy. Subsequently, more understanding of the fuels combustion chemistry is of pinnacle importance. 2-methyl heptane (C₈H₁₈-2) has always been an important component in numerous engine fuels such as JP-4 [1], FACE [2], and S-8 [3]. However, the amount of research dedicated to the study of C₈H₁₈-2 remains minimal. Most of the research of iso-paraffins combustion focused on shorter hydrocarbon chains; starting from iso-butane [4-5], iso-pentane [6-7], and iso-hexane [8-9]. Few studies were performed on 2-methyl heptane [3, 10, 11] focusing on the ignition delay measurements [3], comparison between n-C₈H₁₈ and C₈H₁₈-2 low temperature combustion in a jet stirred reactor [10], and flame speciation in a counter-flow burner [11]. In this research we examine the low-pressure combustion of 2-methyl heptane and one of its isomers 3-methyl heptane. The goal is to identify the major species, intermediate species, as well as isomers in the reaction pool. In addition, identify the effect of the methyl group position in the heptane chain on the combustion chemistry.

Approach

The experiments were demonstrated at the Advanced Light Source (ALS) at Lawrence Berkeley National Laboratory. The ALS provides tunable monochromatic synchrotron radiation in the UV range which is used for gas photoionization. The experimental setup consists of a flat flame stabilized on a McKenna burner placed in a low-pressure chamber. The burner was mounted on a translational stage to allow gas sampling at different axial locations. The gas was sampled using a quartz nozzle then injected into a molecular beam chamber. The formed molecular beam was, then, subjected to the synchrotron radiation for ionization. The ionized stream was then introduced into a time of flight mass spectrometer with a mass resolution of $m/\Delta m \sim 3500$. Different ionization energies were used so as to identify species with different ionization threshold. The flame was stoichiometric with 50% dilution with argon, while the fame chamber pressure was 20 torr. Numerical comparisons were performed using the reaction mechanism of Sarathy et al. [11].

Results and discussion

Figures 1 and 2 present the mole fractions of the major products of C₈H₁₈-2 and C₈H₁₈-3 flames, respectively. No major differences were noticed neither from the quantitative nor the qualitative point of view. Similarly, the trends of the C₂ and C₃ intermediate hydrocarbons did not show a major difference in their trends between both flames. Figure 3 and 4 show the isomers of C₄H₈ formed in both

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flames. Formation of 1-butene was evident in both flames. However, the formation of iso-butene was only limited to the 2-methyl heptane flame. On the other hand, formation of 2-butene was attained only in 3-methyl heptane. These differences are attributed to the difference in methyl group position in both fuels.

Conclusions

Investigations of 2- and 3-methyl heptane laminar premixed flames at low pressure were conducted using VUV photoionization mass spectrometry. Results did not show prominent differences of the major products of both flames. However, significant differences were observed on the isomers and intermediate species starting from C4. Energy scans and literature results were used for the calculation of mole fractions of all isomers.

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Figures

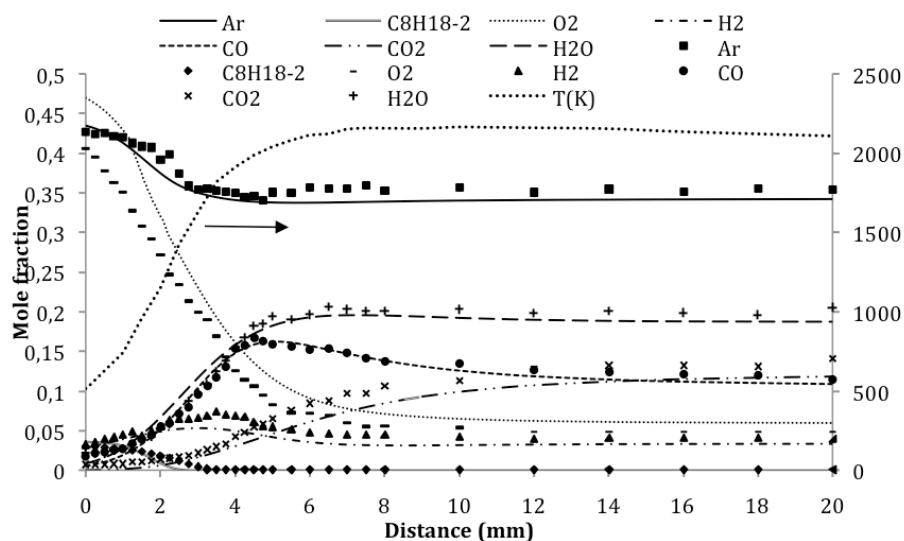


Figure 1. Major species obtained in C_8H_{18-2} flame, experimental (symbols), lines (numerical).

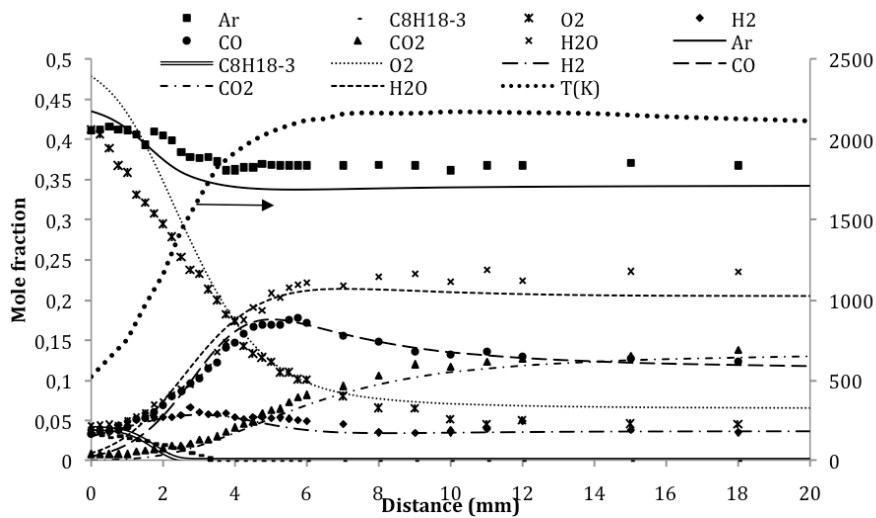


Figure 2. Major species obtained in C_8H_{18-3} flame, experimental (symbols), lines (numerical)

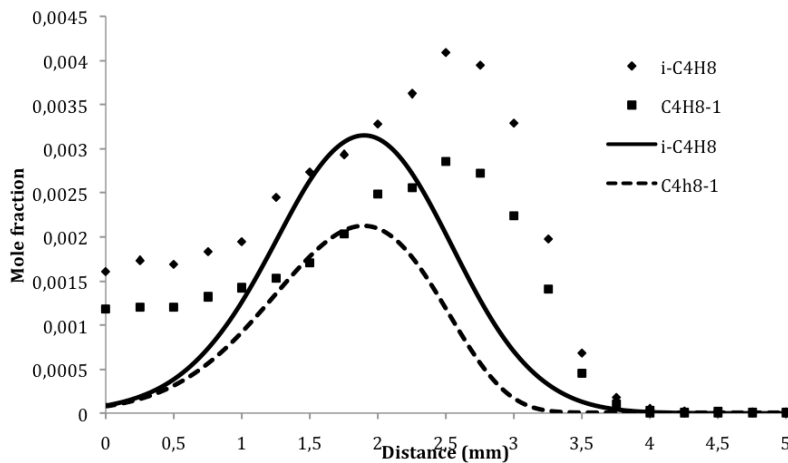


Figure 3. C_4H_8 mole fractions in C_8H_{18-2} flames, experimental (symbols), lines (numerical)

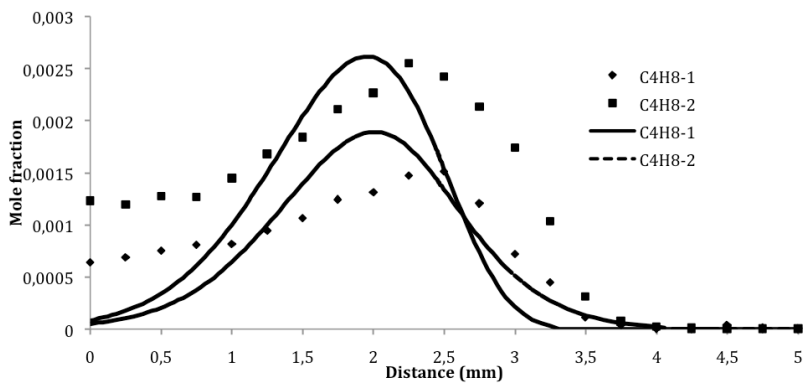


Figure 4. C_4H_8 mole fractions in C_8H_{18-3} flames, experimental (symbols), lines (numerical)

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