Comparing the Influence of Propane and n-Heptane Addition on Methane Ignition at High Pressure

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Introduction

In a theoretical study, the influence on the ignition delay time of propane and n-heptane addition to a mixture of methane and air at a pressure value of 60 bar was investigated. Increasing the propane content in a methane-propane mixture leads to a decrease of the ignition delay time, but at the same time the formation of a negative temperature coefficient (NTC) region [1] can be observed. Using n-heptane instead of propane, a lower amount of additive is necessary to gain a similar ignition delay time reduction over a certain temperature range. This is the basis to optimise the gas composition.

Methodology

The ignition properties of a methane-air mixture was modified by the addition of propane and n-heptane, respectively. This theoretical investigation was performed with the software LOGEsoft v1.08 by using the recently released and very detailed n-heptane mechanism by Zhang et al. [2] with 1268 species und 5336 reactions.

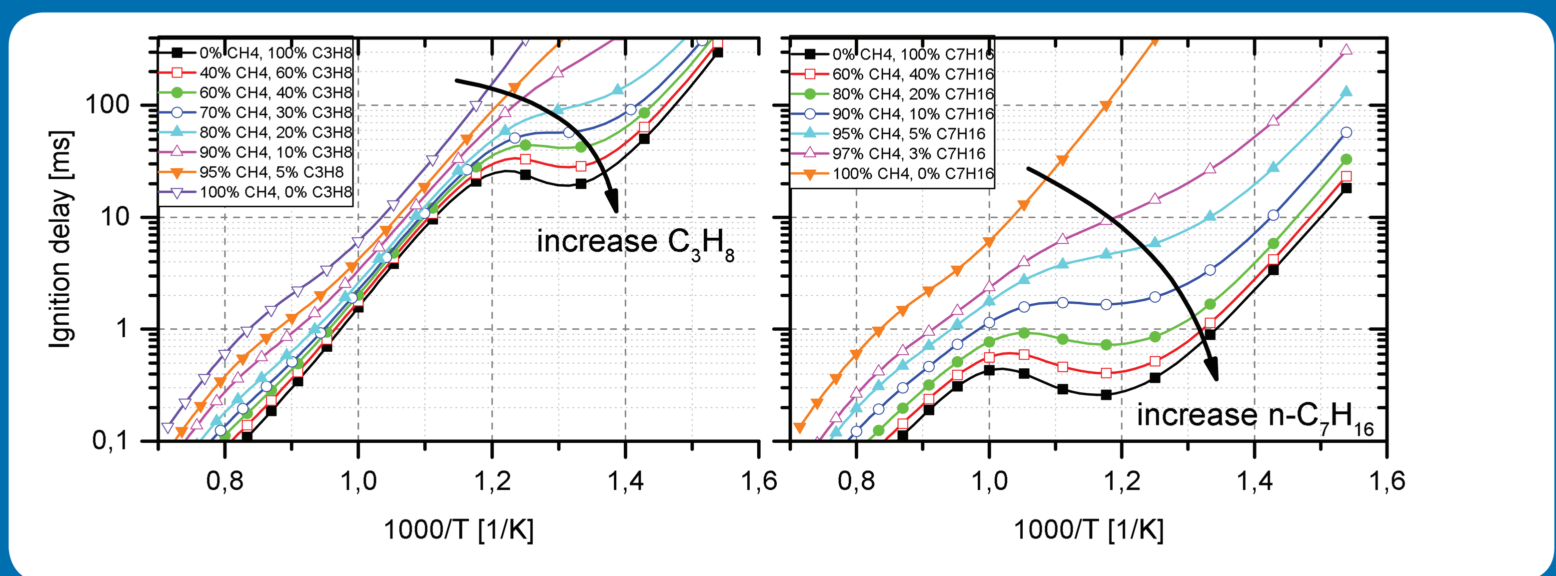

Figure 1: Ignition delay time of methane-propane-air (left) and methane-n-heptane-air mixture (right) with changing fuel composition, $\lambda = 1.6$ and $p_{start} = 60$ bar.

Figure 1 shows the influence of adding propane (left) and n-heptane (right), respectively, to the methane-air mixture. Additionally a sensitivity analysis was performed with LOGEsoft [3]. Three different gas mixtures with an air to fuel ratio of 1.6 and a starting pressure of 60 bar were chosen: 40 vol% methane and 60 vol% propane, 80 vol% methane and 20 vol% n-heptane, 97 vol% methane and 3 vol% n-heptane. Figure 2 shows the chronological sensitivity sequence of the gas mixture with 40 vol% methane and 60 vol% n-heptane at 780 K as an example. The ignition delay time as function of the temperature of all three gas mixtures is shown in the upper part of Figure 3.

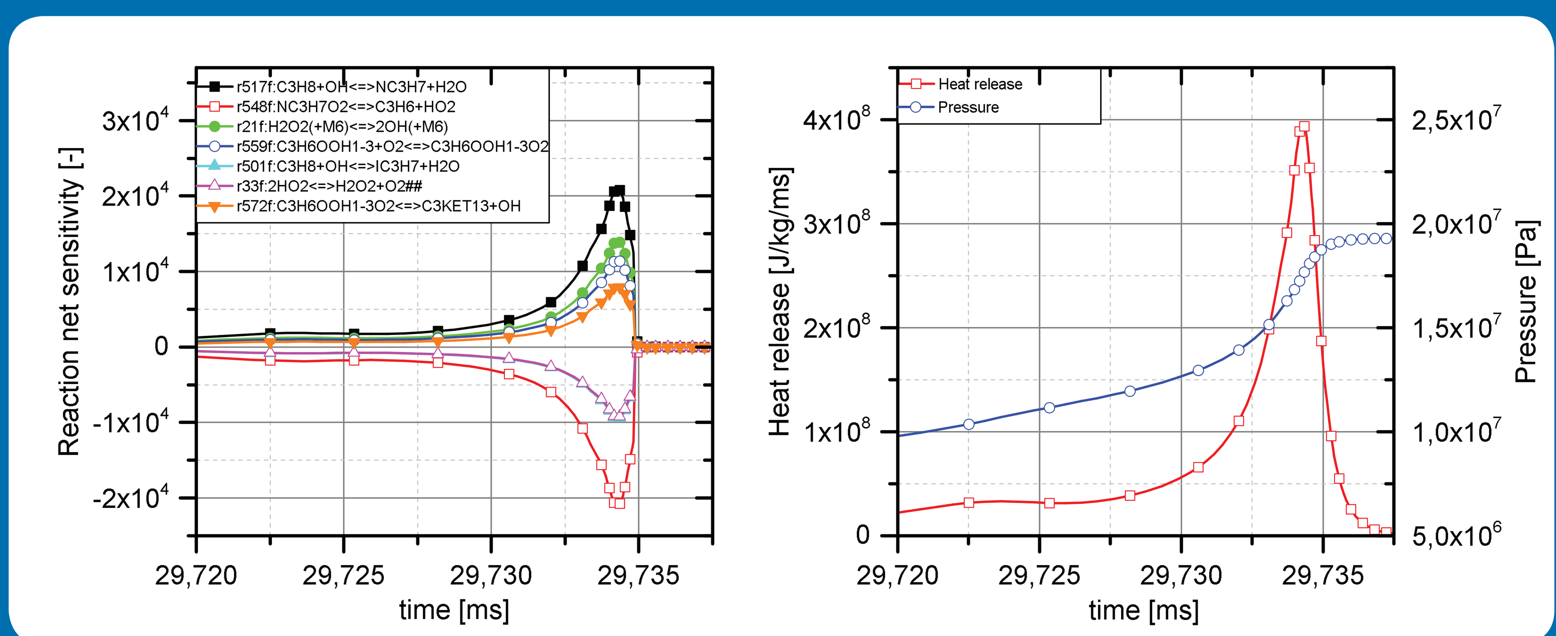

Figure 2: Chronological sequence of reaction net sensitivity towards temperature of the gas mixture 40 vol% methane and 60 vol% propane with $\lambda = 1.6$, $p_{start} = 60$ bar and $T_{start} = 780$ K (left); Released heat and pressure gradient during the ignition process (right).

Results

By doping the methane-air mixture with hydrocarbons with a higher carbon number, a reduction of the ignition delay time can be achieved. Due to the fact that compared to propane already a small amount of n-heptane is sufficient for reducing the ignition delay time significantly, the doping process can be applied without causing a NTC regime. At a temperature higher than 1100 K, the addition of 20 vol% n-heptane leads to the same reduction of the ignition delay time as the addition of 60 vol% propane. At a temperature below 740 K, the required amount of n-heptane is 3 vol% to gain the same ignition delay time reduction as by the addition of 60 vol% propane.

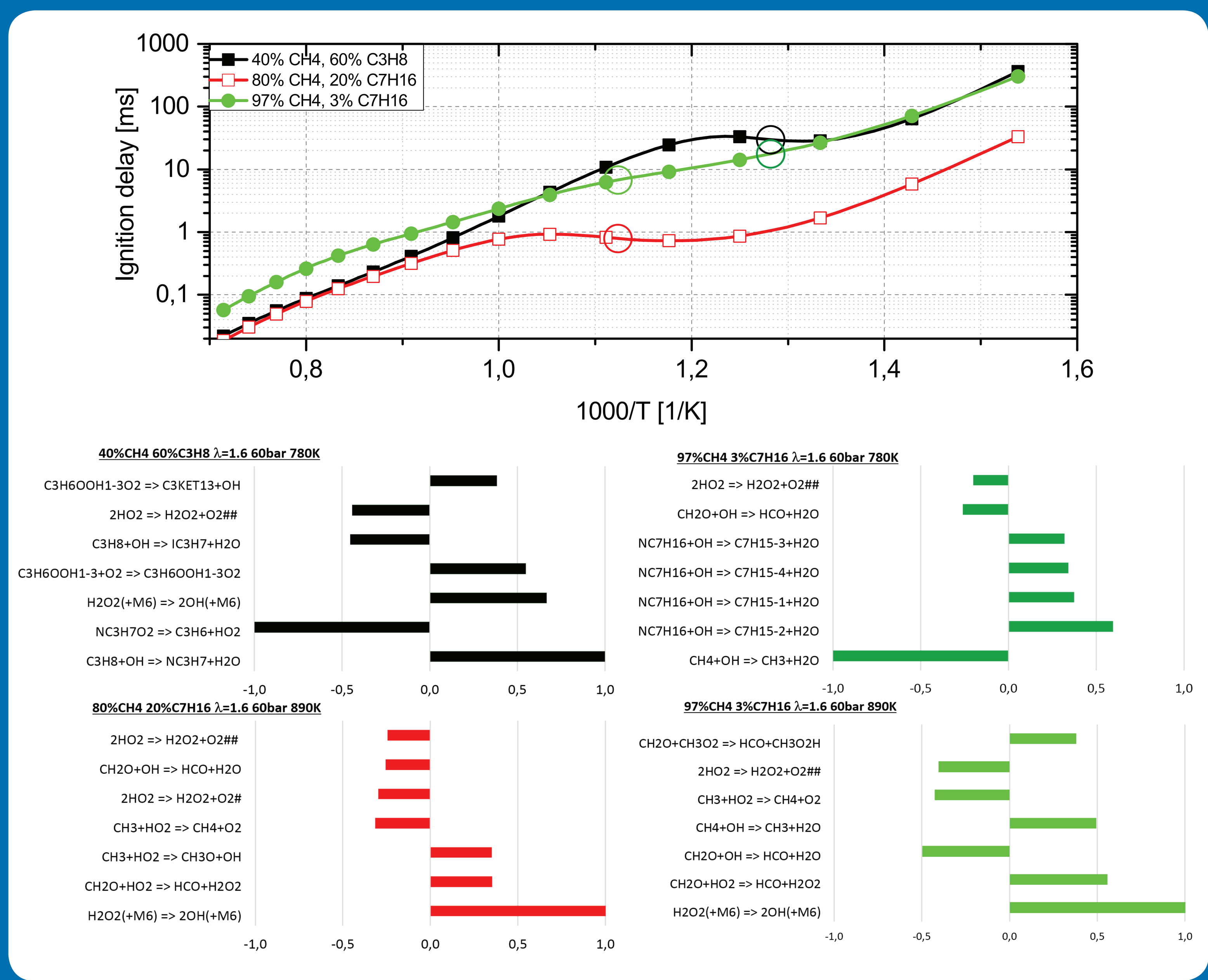

Figure 3: Ignition delay time of the three investigated gas mixtures (top); Normalised reaction net sensitivity (bottom). The coloured circles in the upper diagram indicate the parameter configuration for the performed sensitivity analyses.

Acknowledgements

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References

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[2] K. Zhang, C. Banyon, J. Bugler, H.J. Curran, A. Rodriguez, O. Herbinet, F. Battin-Leclerc, C. B'Chir, K.A. Heufer, An updated experimental and kinetic modeling study of n-heptane oxidation, Combustion and Flame 172 (2016) 116-135.

[3] LOGEsoft manual, Book 5, LOGE AB Lund, 2016.

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