Simulating the flame velocity of methane- and n-heptane-air mixtures with a reaction mechanism for dual fuel combustion and further mechanism optimization by comparison with experimental data

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Introduction

Reduction of pollutant emissions from large engines, as used in shipping, can be achieved by changing over to dual fuel engines using the combination of diesel and natural gas. To optimize the operation of a dual fuel engine, detailed investigations on an engine test bench are necessary. However, the operation of such test stands is associated with high costs. A way of reducing the costs is the utilization of simulation tools with an appropriate reaction mechanism. Although these tools cannot replace the application of engine test benches completely, it is possible to reduce the total engine development costs by a smart combination of simulation and experiment. In this study, a reaction mechanism adapted for dual fuel operation is analyzed with focus on the laminar flame velocity calculation.

Reaction mechanism for dual fuel operation

Dual fuel combustion represents a very complex burning process due to the presence of inhomogeneous distributed large hydrocarbons of the diesel fuel and small hydrocarbons of the natural gas in the combustion chamber. For the theoretical investigation of this combustion process, it is therefore necessary to use a mechanism that correctly reproduces the interactions between the different fuel types. Based on the San Diego Complete Mechanism [1] with the n-heptane and NOx extension, a mechanism adapted for the simulation of a dual fuel burning process has been presented in a previous study [2]. The validation of this mechanism was performed by comparing calculated and measured ignition delay times of methane/propane and methane/n-heptane mixtures. In addition to the correct calculation of the ignition timing, the proper determination of the propagation velocity of the flame front in the combustion chamber is of great importance.

Laminar flame speed calculation and validation

The study presented here deals with the simulation of the laminar flame velocity with the dual fuel mechanism using the software LOGEresearch [3]. An analysis was made by comparing the calculated flame velocities for methane (surrogate for natural gas) and n-heptane (surrogate for diesel) with experimentally determined values. A literature review has shown that hardly any or no adequate data of experimental investigations of flame speeds at a pressure value in the range of 100 bar and higher are available. Therefore, two different strategies for mechanism validation were used. In the low-pressure range (up to 25 bar), available experimental data [4-6] were used for the mechanism validation. In the high-pressure range (100 and 150 bar), a comparison of the simulation results of the dual fuel mechanism with results from established mechanisms [7-10] was performed. The comparison has shown that the laminar flame velocities calculated with the dual fuel

mechanism are already of the correct order of magnitude. In dual fuel operation, a flame front spreads into the gas-air mixture after ignition with a diesel jet. Therefore, the flame propagation in a methane-air mixture was investigated in detail as a next step. The flame velocities of methane-air mixtures were simulated in the range $0{,}5 < \phi < 1{,}4$ at a pressure value of 1, 5 and 10 atm, followed by an comparison with experimental values [5]. The study revealed an overestimation of the laminar flame velocities for $\phi \lesssim 1$ as shown in Figure 1.

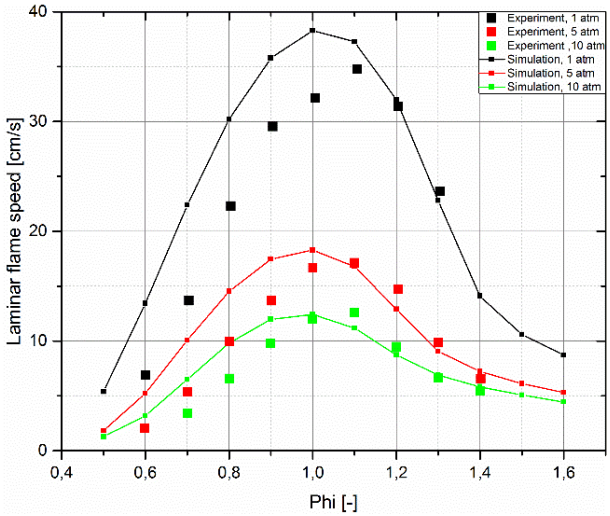

Figure 1: Measured and calculated laminar flame velocities of methane-air mixture at a pressure of 1, 5 and 10 atm, gas temperature of 299 K and a fuel-air equivalence ratio between 0,5 and 1,6.

To determine which elementary reactions have a major impact on the resulting flame velocity in the lean region, a sensitivity analysis was carried out for a fuel-air equivalence ratio between 0,5 and 1,4. Since a methane-air mixture was investigated, methane was used as the target species for the analysis. As a result of the sensitivity analysis, $H + O_2 \leftrightarrow OH + O$, $CO + OH \leftrightarrow CO_2 + H$ and $H + CH_3\,(+M) \leftrightarrow CH_4(+M)$ were identified as suitable elementary reactions for the laminar flame speed adjustment. The adaption was performed by changing the Arrhenius coefficients of the respective elementary reactions. Table 1 gives an overview of the Arrhenius coefficients in its configuration before and after the adaption process.

Table 1: Overview of the adapted elementary reactions and the adjustment of the Arrhenius coefficients.

Reaction	**Parameter status**	$\boldsymbol{A}\,[-]$	$\boldsymbol{\beta}\,[-]$	$\boldsymbol{E_A}\,[\boldsymbol{cal/mol}]$
$H + O_2 \leftrightarrow OH + O$	before	$1{,}00 \cdot 10^{16}$	$-0{,}70$	11942,29
	after	$6{,}00 \cdot 10^{16}$	$-0{,}70$	17069,79
$CO + OH \leftrightarrow CO_2 + H$	before	$4{,}40 \cdot 10^{6}$	1,50	$-740{,}92$
	after	$1{,}00 \cdot 10^{6}$	1,50	$-740{,}92$
$H + CH_3\,(+M) \leftrightarrow CH_4(+M)$	before	$1{,}27 \cdot 10^{16}$	$-0{,}63$	382,89
	after	$3{,}00 \cdot 10^{16}$	$-0{,}63$	382,89

As can be seen in Figure 2, the adaptation of the Arrhenius parameters led to an increase in the laminar flame velocity at low fuel-air equivalence ratio, thus the experimental values are approximated much better throughout the investigated parameter range.

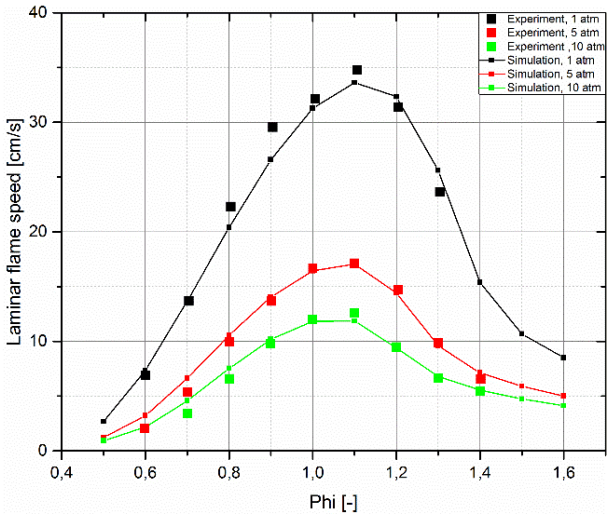

Figure 2: Measured and calculated laminar flame velocities of methane-air mixture at a pressure of 1, 5 and 10 atm, gas temperature of 299 K and a fuel-air equivalence ratio between 0,5 and 1,6 using the reaction mechanism with adapted Arrhenius coefficients.

Influence on ignition delay time

When adjusting the mechanism regarding the laminar flame velocity, care was taken to ensure that the mechanism adaption did not lead to a nameable change in the calculated ignition delay time. Therefore, the ignition delay time was calculated for four different mixtures before and after the mechanism adjustment and was compared with experimental results. The data used for validation were published by Pachler et al. [11] and Herzler et al. [12]. Pachler et al. investigated methane-propane mixtures with a methane-propane mixture ratio of 100 mol% / 0 mol%, 95 mol% / 5 mol% and 70 mol% / 30 mol%. The experiments were performed with a rapid compression machine (RCM) with an end of compression pressure of 100 bar and a fuel-air equivalence ratio of 0,53. Herzler et al. investigated a mixture of 95 mol% methane and 5 mol% n-heptane at a pressure of 30 bar and a fuel-air equivalence ratio of 2 in a shock tube (ST). As shown in Figure 3, the adjustment of the reaction mechanism for adapting the laminar flame speed calculation had no nameable influence on the ignition delay time.

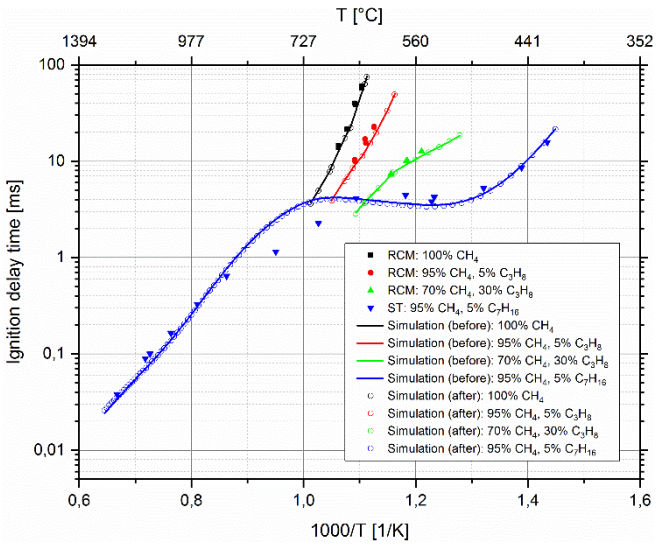

Figure 3: Ignition delay time of methane-propane mixtures and methane-n-heptane mixture simulated with the dual fuel reaction mechanism before and after mechanism adjustment.

Conclusion

A reaction mechanism adapted for dual fuel combustion, developed in a previous study [2], was analyzed regarding the calculation of the laminar flame velocities. Specifically, the propagation velocities of the flame front in methane-air mixtures were considered closely. After an overestimation of the laminar flame velocities was observed in the lean region, the mechanism was adapted by means of sensitivity analysis and adaptation of appropriate Arrhenius parameters of selected elementary reactions resulting in a well approximation of the experimental flame velocities.

Acknowledgement

We would like to show our gratitude to the Austrian Research Promotion Agency (FFG) for funding this work (project number 850690). Further thanks go to LOGE AB for providing the simulation software LOGEresearch.

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