

# Optimization of a Mechanism for Dual Fuel Combustion

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## Motivation and Background

The pollutant emission limit requirements for marine engines and engines used in heavy-duty vehicles like railways and trucks, becoming stricter and more difficult to meet. The operation of engines in dual fuel mode, using the fuels natural gas and diesel, offers the possibility to significantly reduce pollutant emissions. In the development process of a new engine, simulation tools can reduce the required engine test bench time and therefore lower the total development costs. The reaction mechanism used for the simulation must therefore be able to correctly describe both the combustion of natural gas and diesel. In this study, n-heptane was chosen as diesel surrogate, a mixture of methane and propane considered natural gas. As basic mechanism, the Complete San Diego Mechanism with the heptane and nitrogen chemistry add-on was used. In order to reduce the deviation between the simulation results and the experimental values, an optimization of the reaction mechanism was performed. With a sensitivity analysis, influential reactions were identified and adapted by adjusting the Arrhenius parameters to improve the prediction accuracy of the simulation.

## Basic reaction mechanism

The basic mechanism was composed of the Complete San Diego Mechanism and the heptane and nitrogen chemistry add-on [1]. To assess the predictive accuracy of the mechanism, published experimental data for gas mixtures, as well as gas-n-heptane mixtures were used for validation:

- Methane-propane mixtures (Pachler et al. [2]) with variable propane content between 0 and 30 mol% at a pressure of 100 bar and a  $\lambda$ -value of 1.9.
- Methane-n-heptane mixture (Herzler et al. [3]) with 95 mol% methane and 5 mol% n-heptane at a pressure of 30 bar and a  $\lambda$ -value of 0.5

The mechanism analysis (sensitivity and reaction flow), as well as the calculation of the ignition delay time was performed with the software LOGEresearch v1.10 [4].

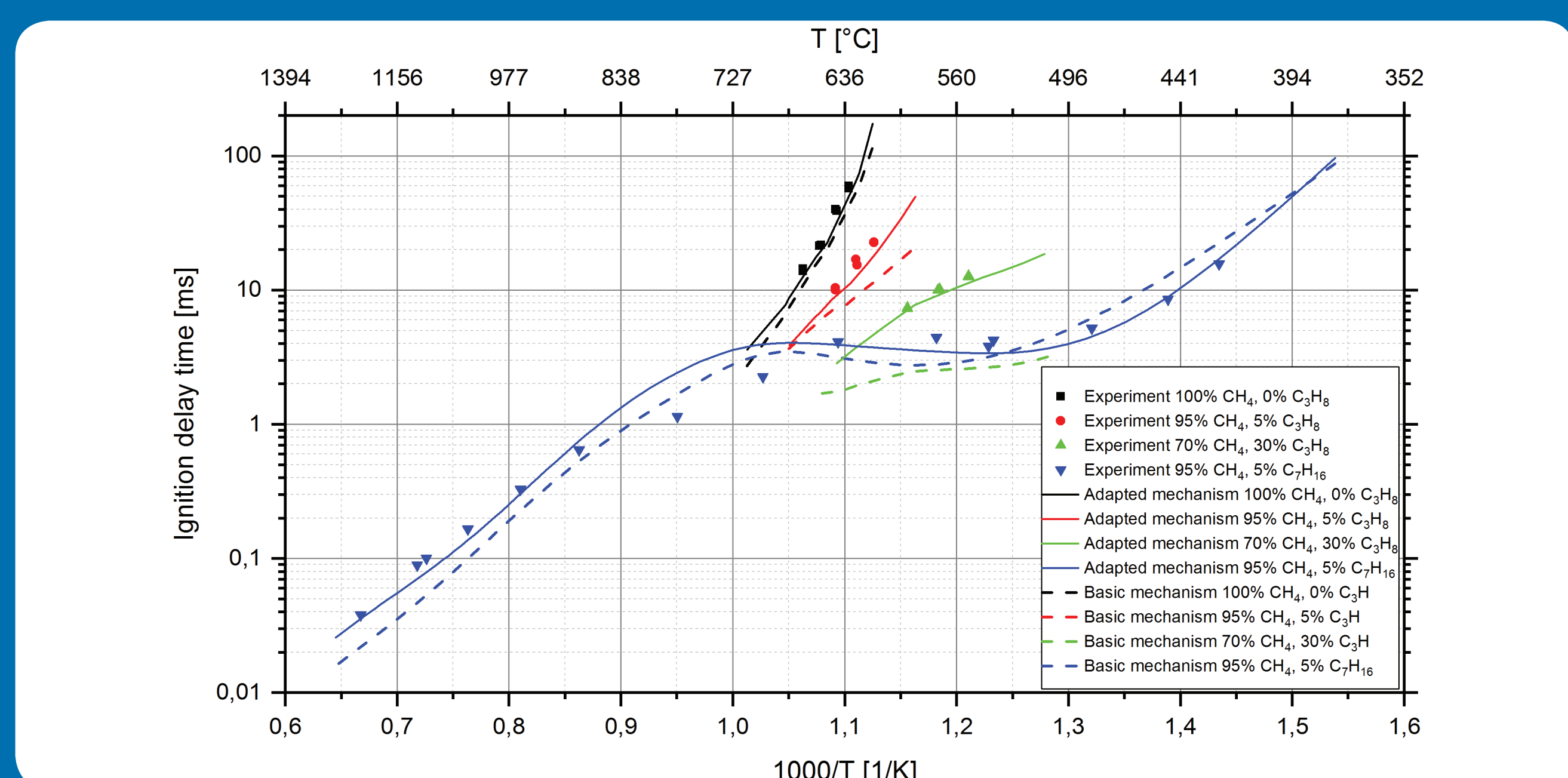


Figure 2: Comparison of experimental data and simulation results using the basic and the adapted reaction mechanism.

## Results

As a result of the mechanism adaptation, the influence of propane addition on the ignition delay time is reproduced well. In the case of the methane-n-heptane mixture, a good approximation of the simulation results to the experimental values is evident both in the temperature range 700 to 900 K and in 1150 to 1500 K as shown in Figure 2. In the temperature range 900 to 1050 K, an overestimation of the ignition delay time is obvious, where further adaption is necessary.

## Acknowledgement

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## References

- [1] „Chemical-Kinetic Mechanisms for Combustion Applications,” San Diego Mechanism web page, Mechanical and Aerospace Engineering (Combustion Research), University of California at San Diego (<http://combustion.ucsd.edu>).
- [2] Pachler, R. F., Ramalingam, A. K., Heufer, K. A. Winter, F., „Reduction and validation of a chemical kinetic mechanism including necessity analysis and investigation of CH<sub>4</sub>/C<sub>3</sub>H<sub>8</sub> oxidation at pressures up to 120 bar using a rapid compression machine”, Fuel 172:139-145 (2016).
- [3] Herzler, J., Fikri, M., Welz, O., Schulz, C., „High-pressure shock-tube study of the ignition of fuel-rich CH<sub>4</sub>/air and CH<sub>4</sub>/additive/air mixtures over a wide temperature range,” 7th European Combustion Meeting, Budapest, Hungary, 2015.
- [4] LOGEresearch v1.10 (<http://www.logesoft.com>.)

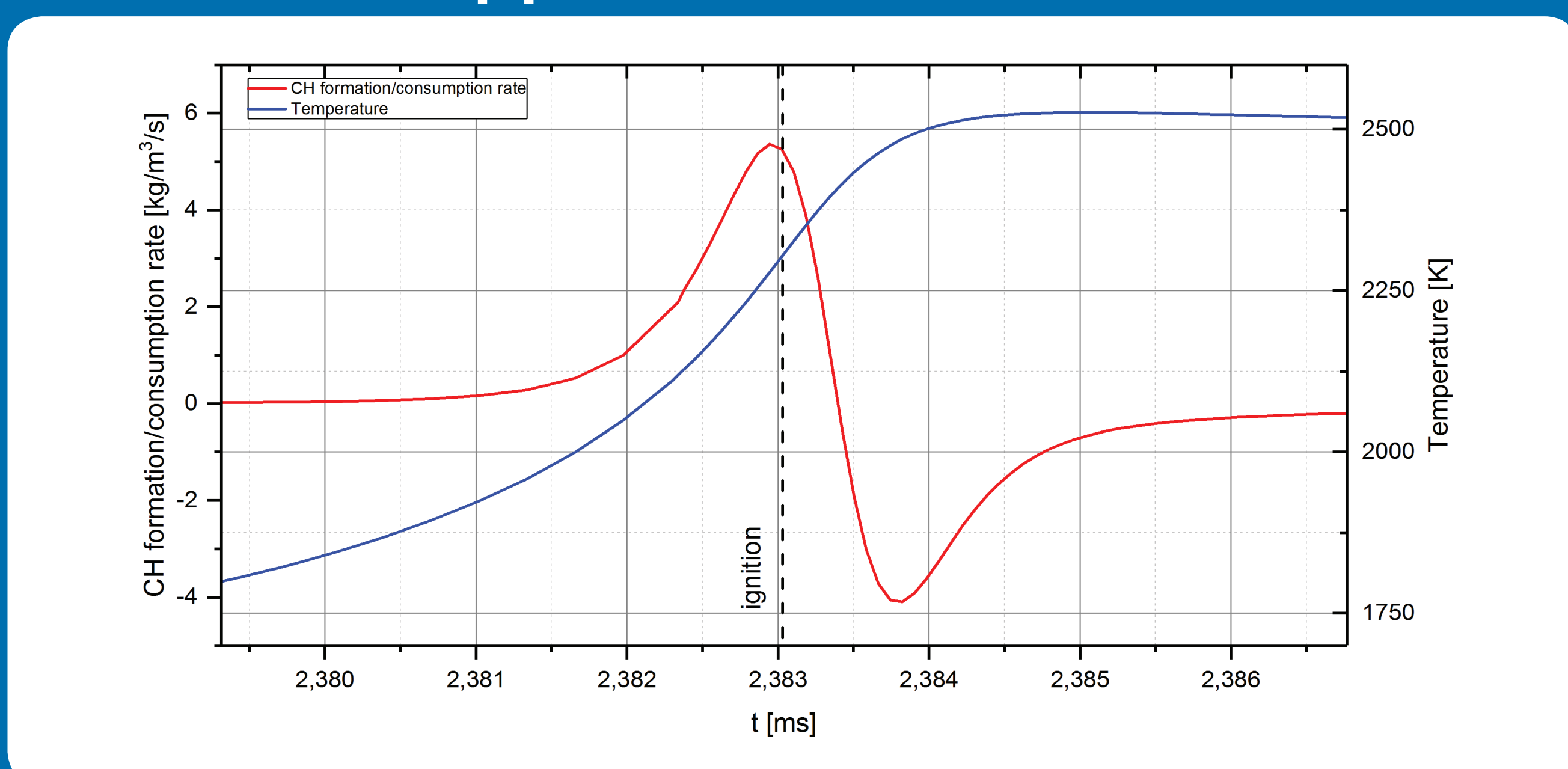


Figure 1: Formation and consumption rate of CH radicals in the range of the ignition point.

## Reaction selection and adaption

The optimization of the mechanism consisted of the following 4 steps:



### 1. Analysing the elementary reactions

The concentration of CH radicals shows a sharp increase shortly before the ignition event as presented in Figure 1 and can therefore be used as an ignition trigger. The elementary reactions were investigated concerning their influence on the formation of CH-radical.

### 2. Selection of elementary reactions for optimization

12 of 354 reactions have been selected for optimizing the mechanism.

### 3. Adaption of reactions

The reactions were adapted by changing the Arrhenius parameters.

### 4. Validation against experimental data

The simulated ignition delay time was compared with RCM- and shocktube measurement data.