

Laminar burning velocities of methylcyclohexane + air flames at room and elevated temperatures

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Introduction

Aviation kerosene or jet fuel is a complex mixture of different classes of hydrocarbons with the major contributors being normal alkanes, branched chain paraffins (iso-alkanes), aromatic molecules and cyclic paraffins, cycloalkanes [1]. Formulation of the proper surrogate fuels reproducing practical (physical) and combustion characteristics of kerosene requires, therefore, detailed understanding of the combustion chemistry of each of these classes. The laminar burning velocity, one of the most important characteristics of combustible mixtures, has been recently investigated in our flame studies of n-heptane [2, 3] and n-decane [4] representing n-alkanes, of iso-octane [2, 3], of aromatic benzene [5] and toluene [2].

Cycloalkanes possess unique combustion features important for oxidation of real fuels [6, 7] and, therefore, the goal of the present study was to measure burning velocities of methylcyclohexane + air flames at room and elevated temperatures. Previously, burning velocity, S_L , of methylcyclohexane was investigated in spherical and counterflow flame configurations. Kumar and Sung [8] obtained S_L at atmospheric pressure and initial temperature of 400 K using the counterflow technique and linear stretch correction. Ji et al. [9] also implemented the counterflow configuration, yet the stretch-correction was performed using so-called computationally-assisted technique. The authors determined S_L at atmospheric pressure and initial temperature of 353 K and found predictions of the JetSurf 1.1 model in a good agreement with their experiments. Wu et al. [10] investigated expanding spherical flames from 1 up to 20 atm and initial temperature of 353 K using non-linear stretch correction. At atmospheric pressure they found reasonable agreement with the data of Ji et al. [9], yet some discrepancies were observed in lean and rich flames. Wu et al. [10] tested JetSurf 2.0 model [11], which moderately overpredicted burning velocities of methylcyclohexane + air flames especially at atmospheric pressure.

The goals of the present collaborative study were: a) to provide new experimental data over an extended range of initial temperatures including conditions visited in the previous studies [8-10]; b) to compare these data with predictions of two models: JetSurf 2.0 [11] and of the mechanism developed at Politecnico di Milano [12]. Experiments have been performed at Lund University and at Samara University using the same technique, the heat flux method, yet on experimental rigs of different design.

Experimental details

The determination of the laminar burning velocity was performed with the heat flux method. The initial temperature (T_g) of the methylcyclohexane + air mixtures was set to 298, 353 and 400 K, and the equivalence ratio (ϕ) was varied from 0.7 to 1.4. The purity of the fuel was above 99%, and the oxidizer was synthetic air (21% O_2 + 79% N_2).

Lund University

The heat flux method allows stabilization of flat adiabatic flames on a perforated burner. The border of the burner plate was kept at a temperature higher than T_g and up to 423K using an oil circuit. The temperature of the oil was set with a circulator bath Julabo MA-4. The working range of the bath is up to 473K. The uncertainty in the oil temperature inside the burner was evaluated to be about 1K. The flow rates of the oxidizer and fuel were set using thermal and Coriolis mass flow controllers, respectively. The heat flux burner was manufactured at Zhejiang University and had 0.5 mm perforation with 0.7 mm pitch. The diameter of the perforated area was around 4 cm, corresponding to the effective surface area of 12.8 cm².

Samara University

At the Samara setup, the burner plate was kept preheated to 368K using water circulator. The burner had a diameter of 3 cm with the effective surface area of 6.891 cm² and it was manufactured in Eindhoven.

Modeling

Several kinetic mechanisms of methylcyclohexane oxidation were found in the literature. In our previous work on benzene and n-decane [4,5], three mechanisms were considered, and it was shown that the detailed reaction scheme developed at the Politecnico di Milano [12] produces best agreement with the experiments. Therefore, it was selected for modeling in the current study. The second reaction scheme considered is the JetSurF 2.0 model, since its versions were used previously [9,10] to model the S_L of methylcyclohexane + air flames at 353 K. Modeling of the premixed free-propagating planar adiabatic flames was performed using ANSYS Chemkin 18 [13]. The influence of the transport properties formulation was tested for the model [12], and the difference in S_L between mixture-averaged and multicomponent formulations was found to be within 1 cm/s, therefore, the simulation results reported in the current study are obtained with mixture-averaged transport formulation and thermal diffusion. The solutions were tested for grid-independence. The number of grid points was 650-750.

Results and discussion

The laminar burning velocity of methylcyclohexane + air flames was determined at atmospheric pressure and initial temperatures of 298, 353 and 400 K. The overall accuracy was around ± 1 sm/s. For the initial temperatures of 353 and 400 K, the results were compared with the literature data [8-10] on Figure 1. The two datasets at 353 K obtained with the heat flux method in Lund and Samara are in close agreement with each other, with the difference in S_L being below 0.7 cm/s for all equivalence ratios except $\phi = 1$. Comparing these data to the literature values from Ji et al. [9] and Wu et al. [10], the present results correspond to Ji et al. [9] in lean mixtures, and to Wu et al. [10] in rich mixtures. At $\phi = 0.9-1.2$, there is an overprediction by around 3 cm/s. At $T_g = 400$ K (Figure 1 (right)), the results from Lund follow the data from Kumar and Sung [12] up to $\phi = 1.2$, with 3 cm/s difference at $\phi = 1.3$.

None of the two kinetic mechanisms tested were found to match the experimental results obtained with the heat flux method. At both initial temperatures, the model of PoliMi [12] tends to overpredict the S_L , by about 3-4 cm/s at equivalence ratio corresponding to the maximal S_L . On the contrary, JetSurF 2.0 [11] underpredicts the experimental results of the present study. The consistency of the trends at the two initial temperatures suggests that the two models and experimental results have the same temperature dependence of S_L .

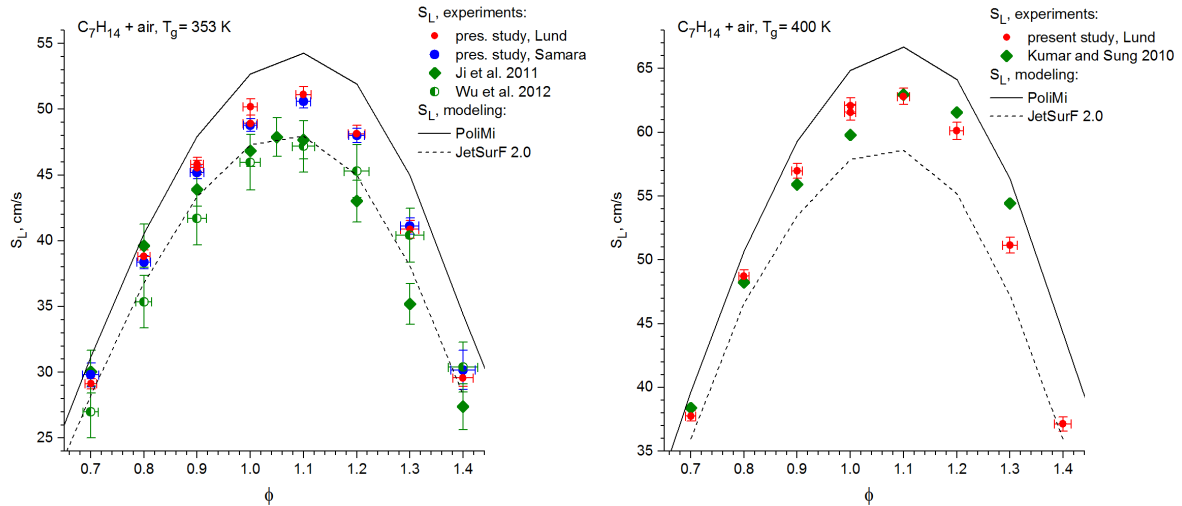


Figure 1. S_L of methylcyclohexane + air at $T_g = 353$ K (left) and 400 K (right). Symbols: experiments, lines: modeling. Present results obtained in Lund (red circles) and Samara (blue circles) are compared to the data of Ji et al. [9] and Wu et al. [10] at 353 K, and of Kumar and Sung [8] at 400 K. The simulations are performed with the PoliMi model [12] and JetSurF 2.0 [11].

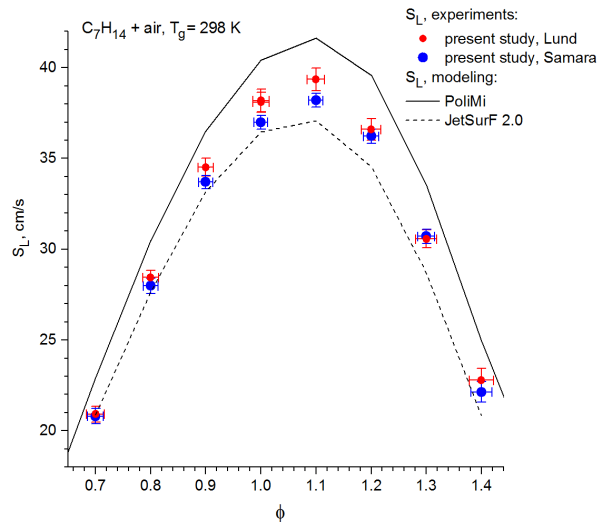


Figure 2. S_L of methylcyclohexane + air at $T_g = 298$ K. Symbols: experimental data obtained in Samara (blue) and Lund (red); lines: modeling.

Finally, Figure 2 presents the new experimental data measured on two heat flux setups in Lund and Samara at room temperature ($T_g = 298$ K). The difference in S_L measured on two setups is within 1 cm/s except for the points $\phi = 1.0$ and 1.1, where it reaches 1.2 cm/s. Comparing the results to the simulations, the same trends can be seen at 298 K as for the two higher temperatures (Figure 1). Also, a common trend between the present results for methylcyclohexane and our previous work on benzene [5] and n-decane [4] can be seen analyzing predictions of the two reaction schemes for kerosene surrogates: PoliMi [12] and JetSurF 2.0 [11]. For all three fuels considered here and in [4,5], calculations with JetSurF give results lower by 5-7 cm/s (at maximal S_L) than those obtained with PoliMi model. The fact that there is a constant shift between the two models which sustains for alkane, cycloalkane and aromatic molecules suggests that the reason for the observed difference lies in the base submechanisms of these two models. This is in line with the sensitivity analysis performed by the authors for benzene + air flames [5].

Conclusions

The laminar burning velocity of methylcyclohexane + air flames was determined with the heat flux method at atmospheric pressure and initial temperatures of 298, 353 and 400 K. The measurements were performed on two experimental setups at Lund University and Samara University, and the results reproduced each other well. The measurements were compared to available literature data and predictions of two detailed reaction schemes developed for aviation fuels – PoliMi [12] and JetSurF 2.0 [11]. Good agreement with Kumar and Sung [8] was observed at 400 K, with slight overprediction of the literature values at 353 K. The two kinetic models disagreed with each other, with the experimental data being located in between the model predictions. The reasons for disagreement between the two models should be looked for in their base submechanisms.

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