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A Chemical Kinetic Investigation on the Burning Velocities of Iso-Propanol/Air Mixtures

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Abstract

The objective of the present study is to develop a detailed chemical kinetic model for describing the combustion behaviour of small alcohols. The focus is on laminar flame speed, one of the major combustion properties. Currently, we are in the process of comparing detailed kinetic modelling results against data gathered from literature and measured in our group.

In the present work, we report on new experimental data on burning velocities of iso-propanol/air mixtures obtained at ambient pressures, for different preheat temperatures, up to 473 K, and at fuel-air ratios ranging φ between about 0.8 and 1.5. The laminar flame speeds were determined in a bunsen-type burner, combined with a pre-evaporator, by applying the cone angle method.

The experimental data are compared with predictions of detailed chemical kinetic reaction mechanisms: Two in-house reaction models were each augmented with an iso-propanol sub model taken from literature [1, 2], and a mechanism published by Dagaut et al. [2].

The suitability of both of the current detailed reaction models will be discussed, also with respect to the predictability of ignition delay times determined recently in our group [3].

Introduction

Over the last years, alternative and renewable energy resources became increasingly important as they contribute to reducing the dependency on fossil fuels and to decreasing CO2 emission.

Alcohols are considered a possible component of alternative fuels and are increasingly used as fuel additive or as fuels in combustion engines. They can inhibit the formation of polyaromatic hydrocarbons (PAH) and soot and improve overall engine performance [4]. For example, ethanol can be produced from cellulosic feedstock and by fermenting sugar or by converting starch. Ethanol is playing a major role within the transport sector, but may also serve for small aircrafts replacing aviation gasoline (avgas) most of the small aircraft engines usually are operated with. For jet turbines, an addition of longer chained alcohols to

kerosene is proposed, in order to meet the strict demands for jet fuels, such as low freezing point or high energy density [5].

A comprehensive understanding of the combustion characteristics of alcohols is important for the development and design of low-emission combustion engines that can effectively use these compounds as fuels or fuel additives. Within this context, the understanding of the combustion pathways of iso-propanol is needed for a

comprehensive description of the oxidation of higher alcohols due to the hierarchical structure of a reaction mechanism.

In the present study, burning velocities of iso-propanol/air mixtures were determined experimentally in a burner combined with a pre-evaporizer by applying the cone-angle method. The values were obtained at ambient pressure and several preheat temperatures, for fuel equivalence ratios of ϕ ranging between 0.9 and 1.6. These data are then used for the development of a detailed chemical kinetic model.

Approach

In the present work, further insight into the combustion behavior of iso-propanol shall be provided. We are focusing on burning velocities as one of the two major combustion properties, besides ignition delay time.

The approach of the present work is to provide experimental data on burning velocities of iso-propanol/air mixtures which will be used for a validation and further optimization of a detailed chemical kinetic reaction model for describing the combustion behaviour for a parameter range typical for the combustion process in a micro gas turbine (T ~1000 -1400 K, p between 1- 4 bar), reflecting the potential in the use of alcohols for the decentralized production of energy.

The laminar high pressure burner concept was developed further towards the use of pre-evaporated liquid fuels. The set-up consists of air fuel supply, burner with flame holder and nozzle, pre-evaporator, and the optional equipment combined with image processing. In addition, a liquid fuel preparation line was built up feeding a thermal evaporator that leads into a fuel conditioning line. From there a mixture preparation line starts opening into the burner eventually. The main components of the fuel/O2/N2-supply are mass flow controllers, high pressure dosing pump, pre-evaporator for the liquid fuel, and mixing chambers. The nitrogen, oxygen, and gaseous fuel flows are mixed at high temperatures.

The values of the burning velocities derived experimentally are compared with those predicted by three chemical kinetic reaction mechanisms. Values of the laminar flame speed were calculated

with the one-dimensional code PREMIX using the preheat temperature determined experimentally and the initial concentrations of the reactants as input parameters.

Results and discussion

First, burning velocities for iso-propanol/air mixtures were determined experimentally in a burner test rig, recently re-constructed for the investigation of liquid fuel-air mixtures. The well-known cone angle method was applied.

Then, these experimental data base was used for the validation and optimization of a detailed chemical reaction mechanism. For this purpose, two in-house reaction models were selected: (i) one called DLR-RG used previously predominantly for predicting ignition delay time data of natural gas, biogenic gas, and syngas mixtures [6]; and (ii) one called DLR-LS mainly used earlier for the calculation of laminar flame speeds of small hydrocarbons [7]. Both reactions models were augmented by an iso- propanol sub model, within the present work.

Reflecting the predictive capabilities of the selected reaction models, two different sub-models were added: (i) for DLR-RG, a sub model was taken from Curran et al. [1], because that sub model was developed for the description of ignition delay times measured in a shock tube; and (ii) for DLR-LS, a sub model from the work of Dagaut

et al. [2] was incorporated because this one was developed for the description of numerous species profiles obtained in a jet-stirred reactor.

The comparison between experimental burning velocities and calculated laminar flame speeds will be presented, as a function of fuel-air ratio and preheat temperature. The mechanisms will be analyzed and discussed.

In addition, the predictive performance of the models with respect to ignition delay time data [3] will also be taken in consideration. Ignition delay data are very important for the development and validation of reaction mechanisms because they describe the global reactivity of the fuel at various mixture compositions, temperatures, and pressures.

Conclusions

Burning velocities of *iso-propanol* in air were determined by applying the cone angle method at ambient pressures and several preheat temperatures, in the fuel equivalence ratio φ between about 0.90 and 1.60.

Existing in-house reaction models were augmented by an iso-propanol sub model taken from literature.

The comparison between burning velocities measured and laminar flame speed data predicted were presented and discussed.

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