Investigations of NO formation in premixed flames of hydrocarbons and alternative fuels

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Combustion plays a crucial role in our energy utilization today and for decades to come. However, to minimize global warming, combustion must take place with a net zero CO_2 emission. This calls for the proper use of biofuels, a renewable and CO_2-neutral option. Using these fuels, however, require an extended understanding of the combustion processes to minimize other pollutants, e.g. NO_x, aldehydes, acids and other toxics, which in turn requires deep knowledge of detailed chemical kinetics of combustion and advanced measuring techniques for model validation crucial for design and engineering.

Although the formation of nitrogen oxides in combustion is sometimes considered well-understood, recent developments revealed significant gaps in our knowledge of the role of many radical intermediates involved in the NO_x formation and reburning. For instance, it is now well realized that the implementation of biodiesel (mixtures of methyl and ethyl esters) leads to increased formation of NOx in the exhaust of car engines. Validation and further development of combustion models for hydrocarbons and alternative fuels require accurate experimental data obtained under well-control conditions. To this end, measurements of nitric oxide, NO, concentrations in premixed laminar flames have been performed using saturated laser-induced fluorescence, LIF.

The present talk will summarize and compare NO formation in premixed flames of hydrocarbons and alternative fuels, namely methane, methanol, n-heptane, ethanol, n-propanol, isopropanol, dimethyl ether, methyl acetate, ethyl formate, and CH_4+NH_3 mixture. These flames have been stabilized at atmospheric pressure and room or elevated initial gas temperature covering equivalence ratios from lean to rich mixtures using the heat flux method that allows for simultaneous determination of their laminar burning velocities. The LIF signal is converted into NO concentration via calibration measurements, which have been performed in flames of methane, methanol and syngas seeded with known amounts of NO. The experimental approach is verified by the measurements of NO concentrations in the post flame zone of methane flames, investigated in previous studies under similar conditions.

Data on the NO formation together with the burning velocities obtained under adiabatic flame conditions provide highly valuable input for model validation, which is illustrated by comparison with predictions of different chemical kinetic mechanisms. The pathways of different NO formation routes and key chemical reactions are discussed with the emphasis on remaining uncertainties in contemporary detailed kinetic schemes for combustion.