Master Thesis
Numerical study of ignition and combustion characteristics of ammonia-hydrogen mixtures

Turbulent combustion is widely used as the energy source in ground and marine transportation, aviation, and stationary power generation worldwide and in Sweden (e.g., Volvo Car, Siemens, etc.), with transition from fossil to renewable fuels being an important trend of the EU and Swedish energy strategies aimed at mitigating the threat of global warming. Among various renewable fuels, carbon-free fuels such as hydrogen H_2 or ammonia NH_3 are of the most interest for reaching the strategic goal of zero CO_2 emissions. While hydrogen burns very well, combustion characteristics of NH_3 are poor. For this reason, ammonia is often considered to be a storage of H_2. Moreover, thanks to excellent combustion characteristics of hydrogen, only a part of NH_3 could be converted to H_2, with the rest being directly burnt as an NH_3/H_2 mixture. Accordingly, basic ignition and combustion characteristics of such mixtures under engine conditions are of great applied interest.

The present project aims at numerically exploring ignition delay times, laminar flame speeds, flammability limits, and other basic characteristics of various ammonia-hydrogen-air mixtures under engine-relevant conditions, i.e., at elevated pressures and temperatures.

The following points should be addressed within the framework of the project:

- Basic characteristics of combustion of a gaseous fuel or a fuel blend,
- Chemistry of combustion of ammonia and hydrogen in air,
- Methods for computing ignition delay time, combustion temperature, laminar flame speed, and flammability limits,
- Physical data required for such numerical studies,
- Experimental data for validation of results of numerical simulations of ignition or/and combustion of NH_3/H_2/air mixtures.

Project description:
More specifically,

- A literature survey will be performed to address the points listed above;
- Software CHEMKIN-PRO will be learnt.
- Several advanced chemical mechanisms of combustion of NH_3/air, H_2/air, and NH_3/H_2/air mixtures will be selected.
- These mechanisms will be tested by running CHEMKIN-PRO and using experimental data found in the literature.
- After selection of the best-in-the-test mechanism(s), it (they) will be used to compute ignition delay times, combustion temperatures, laminar flame speeds, flammability limits, etc. for a wide set of elevated temperatures and pressures by running CHEMKIN-PRO.
- Finally, the obtained results will be summarized in a report and will be presented orally at a seminar.

Suitable background: Studying a master program related to thermodynamics, chemistry, internal combustion engines, or fluid mechanics from, e.g., mechanical, chemical, or automotive engineering. Interest and knowledge in combustion chemistry, ignition, and flames is an advantage, but not a prerequisite. We will learn a lot about combustion chemistry, ignition, and flames during the project.

Thesis level: Master, 20 weeks (30 HP) per student.

Language: English

Starting date: Flexible

Number of students: Two or one.

Miscellaneous: Do not hesitate to contact us if you would like additional information. Please provide covering letter and CV in your application.

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