Master Thesis
Numerical simulations of highly perturbed lean hydrogen-air flames

Premixed or partially premixed turbulent combustion is widely used in ground transportation (e.g., car engines), aviation (e.g., aero-engine afterburners), and stationary power generation (e.g., gas turbines) 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, hydrogen is of the most interest today, because it is a carbon-free fuel, has very good combustion characteristics (high laminar flame speed, wide flammability limits, low ignition energy, etc.), and can be produced utilizing various technologies. To rapidly develop future highly efficient and ultra-clean engines fueled with hydrogen, both experimental and Computational Fluid Dynamics (CFD) tools should jointly be used. However, the utility of CFD tools for research into turbulent burning of lean-hydrogen air mixtures is highly limited due to inability of the state-of-the-art models of turbulent combustion to predict abnormally high turbulent burning rates well documented in such mixtures. The abnormally high turbulent burning rates are commonly attributed to local changes in the mixture composition due to significant differences in molecular diffusivities of hydrogen and oxygen. The most promising approach to development of a model capable for predicting the discussed effect is based on a hypothesis that the burning rate is controlled by local flame zones that are highly perturbed (stretched) when compared to the common laminar flame. Therefore, basic characteristics of such strongly perturbed flames are of great fundamental and applied interest.

The present project aims at calculating basic characteristics of strongly perturbed hydrogen-air flames by allowing for complex combustion chemistry and differences in molecular diffusivities of hydrogen and oxygen. Subsequently, these characteristics are planned to be used as input parameters for numerically modeling experiments with lean hydrogen-air mixtures and for CFD research into engines fueled with hydrogen.

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

- Methods for numerically modeling highly perturbed flames,
- Characteristics of such flames,
- Chemistry of hydrogen combustion,
- Physical data required for numerical studies of highly perturbed flames,
- Validation of numerical results.

Project description:

- A literature survey will be performed to address the above issues.
- Software CHEMKIN-PRO will be learnt.
- Several (e.g. three) advanced chemical mechanisms of hydrogen combustion 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, it will be used to compute basic characteristics of highly perturbed hydrogen-air flames 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.

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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