# Master Thesis
## *Numerical study of autoignition of fuel-air mixtures at elevated temperatures and pressures*

An increase in the compression ratio is well known to improve thermal efficiency of Spark Ignition (SI) engines used in passenger cars. However, a phenomenon known as a knock (noise, pressure waves in the engine cylinder) strongly impedes improving thermal efficiency of an SI engine by increasing its compression ratio. Knock appears at high pressures and temperatures, deteriorates working characteristics of an SI engine, and significantly reduces its durability. Accordingly, research into knock in SI engines is a crucially important task for car manufacturers such as Volvo Car in Sweden.

Although the knock characteristics depend on various effects, it is autoignition (self-ignition) of unburned fuel-air mixture ahead of a flame expanded after spark ignition that is widely accepted to mainly control the onset of knock. Accordingly, study of autoignition of fuel-air mixtures at elevated temperatures and pressures associated with conditions in combustion chambers of modern and future SI engines is of great fundamental interest and of paramount practical importance for car industry and for sustainable development of ground transportation sector.

Early, fundamental research into knock was mainly based on experimental methods. Over the past decade, rapid developments of computer hard and software, numerical methods, and combustion chemistry make simulations of autoignition of a fuel-air mixture feasible even if the complex chemistry (hundreds of species and thousands of chemical reactions) is taken into account.

Accordingly, **the major goal of the present project** consists in studying autoignition of fuel-air mixtures by using advanced computational tools and complex chemical mechanisms.

**Project description:** More specifically,

- A literature survey will be performed to find experimental data on ignition delays of various fuels and fuel blends under various pressures and temperatures.
- Software CHEMKIN-PRO will be learnt.
- Several (e.g. three) advanced chemical mechanisms will be selected.
- These mechanisms will be tested by running CHEMKIN-PRO and using the aforementioned experimental data.
- After selection of the best-in-the-test mechanism, it will be used to compute ignition delays for a wide set of elevated temperatures and pressures by running CHEMKIN-PRO.
- Subsequently, the computed ignition delays will be tabulated or/and approximated.
- 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 and combustion engines is an advantage, but not a prerequisite. We will learn a lot about combustion chemistry and self-ignition 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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