

Ph.D. Offer:

Experimental and numerical investigation for the use of ammonia in Spark-Ignition engines

Description:

This offer is for a Joint PhD thesis between University of Orléans and Vrije Universiteit Brussel (Belgium).

PRISME is a research laboratory of the University of Orléans working on various engineering fields. Its Energy Combustion Engine department is specialized in optimizing efficiency and limiting pollutant emission of engines using an experimental and 1D modelling approach. The Ph.D. student will work on the Combustion and Fuels thematic of the department that especially focuses on the impact of conventional and new fuels:

- On the combustion in the automotive engine whether it is standard or new combustion modes (Downsizing, HCCI, LTC ...)
- On the pollutant emissions.

BURN is a joint research group of the Vrije Universiteit Brussel (VUB) and Université Libre de Bruxelles (ULB). The PhD student will be more specifically related to the VUB part. BURN's objective is to contribute to the development of flexible, energy-efficient and non-polluting energy conversion technologies, to fit a continuously changing energy scenario demanding for environmental friendly, secure and cost-effective solutions. BURN promotes the development of a COMBUSTION 2.0 framework, by means of modern strategies based on high-fidelity experimental techniques and numerical simulations, robust optimisation and uncertainty quantification.

While the optimization of internal combustion engine remains a very important topic, alternative fuels are also a key aspect to achieve significant reduction of CO₂ emissions. As well in a 100% renewable energy system, as in the transition period towards that point, fuels will have the competitive advantage over batteries of higher energy density. A notable exception is hydrogen which became popular through the power-to-gas application. Hydrogen requires specific storage systems to reach adequate volumetric energy density, e.g. compressing or liquefying it with the corresponding complexity. Power-to-gas is one of the element to unlock energy storage in the future renewable energy scenarios and hydrogen will therefore play a major role. An alternative smart H₂ carriers is ammonia (NH₃) that has similar vapor pressure and requires similar handling equipment than propane. Unlike H₂, it can then be stored very easily with a good energy density. In addition to its toxicity, NH₃ presents some challenges for internal combustion engines. It combines a very high auto-ignition temperature and a very low laminar flame speed as well as a promoting effect in the production of nitric oxides.

The objective of this thesis is to explore experimentally and numerically the potential of ammonia for internal combustion engine as a smart energy carrier. Moreover, the kinetics

pathway towards producing nitric oxides will be analyzed and solutions will be proposed to mitigate their impact.

This PhD will be a collaboration between the University of Orléans and the Vrije Universiteit Brussel (BURN Research group). The PhD will be half financed by the labex Caprysses and half by the VUB. A bi-lateral agreement for PhD supervising will be signed.

Tasks/Objectives:

To achieve the objectives of this project, the PhD student will follow two interrelated paths: experimental characterization in optical and metallic engine and numerical analysis with computational fluid dynamics (CFD). Especially, adding hydrogen or methane will affect the flame kernel development and the propagation in turbulent conditions. In the experimental part, performed in PRISME, the laminar spherical combustion vessel will be used to determine the laminar flame speed. Experiments will be then carried out in a metallic single-cylinder engine to evaluate the efficiency and the pollutant emissions in a wide range of operating conditions. Finally, the use of optical diagnostics in an optical engine will be of great interest to investigate the turbulent flame speed and the flame wrinkling of ammonia-hydrogen-air and ammonia-methane-air mixtures.

In the numerical part, developed in VUB, CFD simulations will be performed to analyze in-depth the flame propagation of ammonia with hydrogen. In a first step, the student will validate the kinetic mechanism and the CFD configuration using the experimental data coming from from PRISME. In a second step, the simulations will be performed in an engine geometry to predict engine performances and emissions when using ammonia with hydrogen. The CFD simulations will be performed using the open-source library OpenFOAM and the high performance computing infrastructure available in VUB. Models developed for ignition, initial flame kernel development and flame propagation will be coupled with a detailed kinetic schemes to predict auto-ignition, hence knock tendency. The integration of detailed kinetics will be performed using tabulation of dynamic adaptive chemistry (TDAC). In the numerical step, the student will explore several engine configurations and settings to optimize these results. The optimization step will use non-intrusive methods combined with uncertainty quantification to obtain a robust optimum. Validation will be performed using the single-cylinder SI engine test benches available at PRISME.

Candidate Profile:

M.Sc. in Mechanical Engineering/Energetics (University or Engineering Degree)

Strong skills in Combustion, Fluid Mechanics, Turbulence, and Thermodynamics are required. Strong willing to develop experimental skills in the combustion field. Knowledge about turbulent combustion modelling is required.

Good oral and written communication skills are required to report, to present in congress and write articles for scientific journals. Mobility between the two countries is needed.

IT: Matlab, OpenFOAM.

Conditions:

Start: As soon as possible. Duration: 3 years

Location: Orléans, France and Brussels, Belgium: alternating periods in total of 18 months in each institutions
Net Salary: \cong 1600 € per month + opportunity for extra mission (teaching).

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Burn research group: <http://burn-research.be/>

Prisme: <http://www.univ-orleans.fr/prisme> -

<https://www.youtube.com/channel/UCbfir7Uxh9asZwWD7ZJp0hQ>