PhD position at IFP Energies nouvelles (IFPEN)

Effect of Zero-carbon combustion on lubricant aging and its impact on emissions

Currently, the energy and transport sectors are going through a period of profound change, including awareness of the impact of emissions on the environment and health. In particular, whether for maritime and road transport or for electricity production, the use of zero-carbon compounds such as hydrogen (H_2) and ammonia (NH_3), is a way to limit emissions, not only because of the absence of carbon in their structure and therefore of associated emissions (CO_2, CO, HC and soot), but also through production processes based on renewable resources.
However, these compounds present combustion properties different from those encountered with conventional hydrocarbons. For example, H_2 generates a high heat release rate (HRR) (and therefore a higher maximum pressure and temperature in the chamber), a significant formation of water as a combustion product, and even non-negligible local concentrations of NOx due to very high combustion temperatures. NH_3 has unfavorable combustion properties: narrow flammability limits and low laminar burning speed. Moreover, its alkaline character and the presence of nitrogen in its structure affect respectively the compatibility of materials and the formation of nitrogen oxides in the combustion system. Despite these aspects, the use of ammonia as a fuel is becoming increasingly attractive for its energy density and easier storage than H_2.
These unconventional combustion characteristics can impact the lubricant properties, through potentially higher thermal and chemical stress and increased contamination with oxidizing components such as nitrogen oxides. In addition, the extreme thermal stresses due to higher temperatures (and lower H_2 sticking distance) can lead to deterioration of viscosity properties or deposit formation, and thus increase the contribution of the oil to particulate emissions. The evolution of lubricant performance over time is highly dependent on its resistance to oxidation and aging in the liquid phase.
Although the combustion properties of H_2 and NH_3 are very different, as much as their chemical character, the comparison of their effect on the properties of the lubricant and on its aging will bring essential elements of understanding to better know the adequacy oil/zero-carbon combustion system.
In this context, the objective of our thesis topic is focused on the understanding of lubricant aging and its impact on particulate emissions in the case of engine combustion with zero-carbon fuels. The experimental approach, detailed in the "Research Strategy" section, aims at investigating the descriptors of the degradation mechanism of the lubricant's physico-chemical properties, and its impact on the formation of particles. This thesis will bring elements of understanding and essential data for the choice, or even the formulation, of lubricants for zero-carbon motorizations, and their line with air quality.

Various studies, mainly in diesel engines, have shown how particulate emissions are impacted by the lubricant, but even for conventional fuels, the impact of the lubricant chemistry is not clear. It is difficult to conclude on a universal trend depending on the type of oil (synthetic, semi-synthetic or mineral). Sulfur content, viscosity, volatility, as well as the content of certain metallic compounds present in the additives, such as calcium, seem to be the factors to be further investigated. In addition, the aging of engine oil also directly impacts the combustion process. Different studies have shown how lubricant aging can increase the propensity for LSPI, due to oil and additive degradation and contamination by wear metals, especially Fe and Cu.
In addition, engine oil is composed of a set of additives, including inorganic compounds, which can also affect the aging of the lubricant under specific conditions such as H_2 or NH_3 combustion, for which there are still very few studies.
The complexity and the different parameters involved in the oil/combustion system matching, show the challenge that remains behind the need to know and control these phenomena that come into play in the role of the lubricant, especially for systems including new zero-carbon fuels. The originality of this thesis is to contribute to improve the knowledge, not very consistent until now, on the interaction of oil with the combustion of zero-carbon fuels. Its interest lies in the characterization of the aging of the lubricant for these new combustions, and its role in the formation of polluting emissions.

The research strategy envisaged for the duration of the thesis consists into 3 main phases.
The first phase will be devoted to the construction of the lubricant matrix. As already said, the knowledge of this problem in the H_2 and NH_3 thermal engine is very little consistent. This phase will be important for the candidate to consolidate his knowledge on the aging of the lubricant. The output of this investigation will allow to constitute the lubricant matrix that will include variations of additives and chemical components to investigate and possibly also bio-oils.
The second phase will be the experimental phase of the thesis and will consist of two parts. The part "Characterization of the evolution of the lubricant matrix" has as objective to study in a controlled way the ageing of oils in a closed reactor, and to analyze its properties before and after ageing. For this, the doctoral

student will have to set up various techniques and experimental devices ranging from analyzes of physico-chemical properties, mass spectrometry and IR in oil samples aging reactors. On the other hand, the impact on combustion and on emissions will be the subject of the second part "Experimentation under engine conditions", where the phd student will characterize solid and gaseous emissions from engine test. This will be done at Prisme Laboratory (University of Orléans) during one year.
In the third part, based on the descriptors identified in phase 2, a phenomenological model will be proposed to describe the degradation of the physico-chemical properties of the oil and its impact on the formation of particles during the combustion of these decarbonated fuels. Furthermore, this thesis project will provide essential data and understanding for the development of analytical techniques adapted to the characterization of oils and the impact of decarbonized combustions on air quality. The originality of the subject will allow the selected candidate to interact with experts from different fields.

Keywords: Lubrication, pollutant emissions, combustion, hydrogen, ammonia.

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Doctoral School	ED 552 EMSTU, https://collegedoctoral-cvl.fr/as/ed/CDCVL/index.pl#
PhD location	IFP Energies nouvelles, Rueil-Malmaison, France
Duration and start date	3 years, starting in fourth quarter 2022
Employer	IFP Energies nouvelles, Rueil-Malmaison, France
Academic requirements	Master's degree in Chemical Physical sciences or Chemical Engineering
Language requirements	Fluency in English, and in French or willingness to learn French
Other requirements	Knowledge of the field of combustion and a strong taste for experiments.

To apply, please send your cover letter and CV to the supervisors indicated here above:
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About IFP Energies nouvelles

IFP Energies nouvelles is a French public-sector research, innovation and training center. Its mission is to develop efficient, economical, clean and sustainable technologies in the fields of energy, transport and the environment. For more information, see our WEB site.
IFPEN offers a stimulating research environment, with access to first in class laboratory infrastructures and computing facilities. IFPEN offers competitive salary and benefits packages. All PhD students have access to dedicated seminars and training sessions. For more information, please see our dedicated WEB pages.

About PRISME Laboratory

The research institute, PRISME (UPRES 4229) of the University of Orléans aims to provide a consistent scientific strength of Complex Systems Engineering. The Energy, Combustion and Engine lab (ECM) has the expertise to carry out experiments on optical and metallic single cylinder research engines and on high pressure/high temperature vessels and coordinates and participates to several ANR projects. Pr. C. Rousselle studies ammonia and ammonia/hydrogen combustion for 5 years and is involved on two H2020 projects related to ammonia combustion (FlexnCOnfu and ARENHA) see our Web site (www.univ-orleans.fr/PRISME/ECM).