Ph.D. Position: Experimental and modelling studies of ether oxidation

Subject :

Current transportation fuels are derived from petroleum and their partial replacement using renewable products derived from biomass is being considered in all industrialized countries and is on EU's agenda. The goal is to reduce dependence on oil and limit carbon dioxide emissions (greenhouse gas). In order for these biofuels to be considered as viable alternatives to conventional fuels, it is essential to have a very detailed knowledge of their combustion kinetics. In-depth studies of overall reactivity and detailed oxidation, and in particular the nature of the pollutants formed, are therefore necessary.

Among these biofuels, ethers have recently turned out to be very interesting. For example, diethyl and di-n-butyl ether can be produced via lignocellulosic biomass (2nd generation) and have high cetane numbers which gives them the advantage of being able to be blended with diesel. Our previous studies [1,2] in jet-stirred reactor demonstrated the very high reactivity of these fuels at low temperatures (~450 K). The same studies also show negative temperature coefficient behavior over two temperature intervals for di-n-butyl ether, not observed before with any other fuel. These results have highlighted the complexity of the low temperature kinetics of these compounds, which deserves to be investigated in depth.

In this thesis, we will study the oxidation kinetics of ethers from two aspects: (i) experimental studies and (ii) kinetic modeling. The experimental aspects will include a part which will be realized in ICARE using a jet-stirred reactor, in order to obtain detailed data such as the molar fractions of the products formed during oxidation as a function of temperature. This study will complement the results already obtained at ICARE on the oxidation and pyrolysis of diethyl ether, di-n-propyl ether, di-iso-propyl ether and di-n-butyl ether. The second experimental part will be realized in PRISME using a rapid compression machine in order to measure auto-ignition delays under temperature and pressure conditions close to engine operation, but using diluted mixtures because of the very high reactivity of the ethers. A detailed kinetic mechanism will be developed during this thesis to represent these results. This mechanism will be integrated to the mechanisms developed in ICARE.

In addition to this, a collaboration with the Combustion Chemistry Center (C3) of NUI Galway is envisaged. The PhD student will therefore have the possibility of carrying out ignition delay measurements in a high-pressure shock tube, extending the domain of this study to high temperatures, necessary for model validation. Even if some studies exist in the literature on the oxidation of ethers, these are much less numerous compared to other biofuels such as alcohols for example, even though the mechanisms involved in ether oxidation reveals to be more complicated. There is a lack of experimental data and there are gaps in the understanding of the kinetics. With this thesis, we will carry out a systematic study on selected cyclic and non-cyclic mono-ethers in order to better characterize this family of molecules. Experimental results obtained in this study will be a first in the literature, as well as the kinetic mechanism. This project contributes to environmental protection since the fuels considered should help reduce both fossil fuel dependence and CO_2 emissions while encouraging technological innovation.

The selected candidate will have a three-year doctoral contract, conditioned by a re-registration each year to the graduate school. The monthly stipend is about 1400 euros net monthly. The student is encouraged (in addition to his PhD research) to do teaching, which increases the monthly income to

approximately 1650 euros net. Both laboratories are located in Orléans (France), a medium-sized student city close to Paris. The student will have the possibility to attend international conferences and meetings during his/her PhD.

Keywords : biofuels, combustion, ethers, oxidation, jet-stirred reactor, rapid compression machine

Conditions

Start : October 2020

Duration: 3 years

Location: Orléans (Laboratoires ICARE and PRISME), France

Net Salary: 1420€ / month, opportunity for 1660€/month with extra missions (e.g. teaching)

Contact :

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[1] S. Thion, C. Togbé, Z. Serinyel, G. Dayma, P. Dagaut, *A chemical kinetic study of the oxidation of dibutyl-ether in a jet-stirred reactor*, Combustion and Flame, 185 (2017) 4-15.
[2] Z. Serinyel, M. Lailliau, S. Thion, G. Dayma, P. Dagaut, *An experimental chemical kinetic study of the oxidation of diethyl ether in a jet-stirred reactor and comprehensive modeling*, Combustion and Flame, 193 (2018) 453-462.