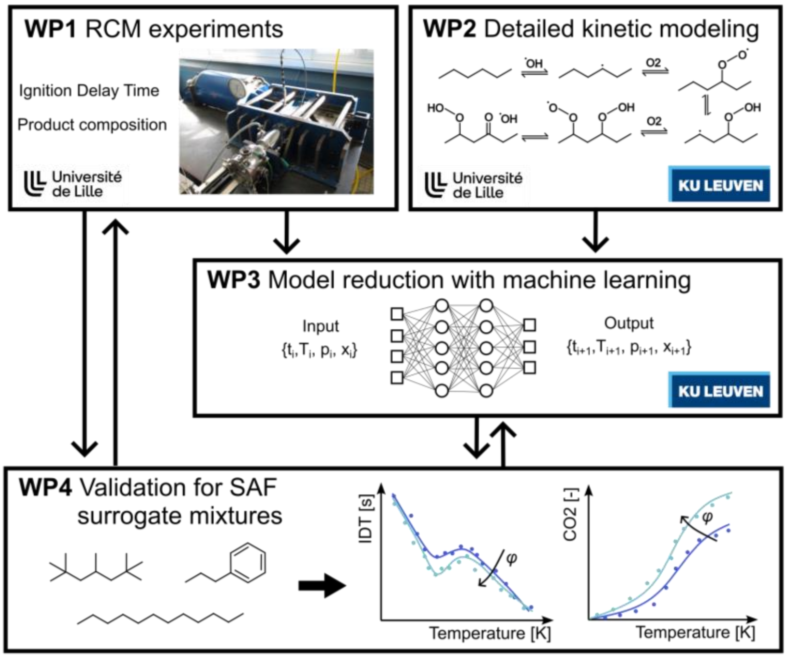
PhD position in PC2A (CNRS/Université de Lille) and CREaS (KULeuven)

Combustion of Sustainable Aviation Fuels: From experiments to robust and accurate reduced kinetic models



Combustion-driven processes are still responsible for a large proportion of energy production and conversion worldwide. **Aeronautic transport**, especially, **is one of the fastest-growing emission sources of Greenhouse Gases**, causing sustainability concerns. Because aircraft electrification is not realistic in the coming decades, Sustainable Aviation Fuels have emerged as an immediate improvement in terms of climate change impact. The introduction of such fuels relies heavily on the possibility to model their combustion chemistry within the Computational Fluid Dynamics codes used in the industry. The chemical structure of such fuels, along with the wide range of temperatures, compositions, and pressures relevant to combustion in gas turbines, imposes the use of **detailed kinetic models** that contain tens of thousands of elementary reactions involving thousands of species. This results in unrealistically computationally expensive simulations, and has motivated the development of kinetic model **reduction strategies** for conventional (fossil-based) Jet-A fuels.

These strategies, however, frequently result in a loss of the predictive ability of the models. This project aims at developing, for the first time, robust and accurate kinetic models for Sustainable Aviation Fuels by means of a **novel approach** that integrates **experiments**, **kinetic modeling**, and **machine learning**. This approach benefits from the unique combined expertise of the ULille group in experimental work and kinetic modeling, and of the KULeuven group on kinetic modeling and machine learning. Experiments will be performed in Lille using a Rapid Compression Machine in the Low Temperature Combustion regime to validate detailed kinetic models for pure components as well as surrogate mixtures. These detailed kinetic models will then be used to train a ML model with a transfer learning methodology.

This project benefits from a **4-year PhD grant** in co-direction between ULille and KULeuven, with stays in both labs over the grant's duration, for an approximate duration of 3 years in Lille and 1 year in Leuven.

Keywords: Sustainable Aviation Fuels; Combustion chemistry; Kinetic modeling; Machine&Transfer Learning; Ignition delay.

Academic Requirements: A Master's degree or an Engineering Degree in the fields of Chemistry, Chemical Engineering, or Mechanical Engineering and a taste for experimental work and computation are required. Additional knowledge in the fields of combustion chemistry will be beneficial.

Doctoral School: ED Sciences de la Matière, du Rayonnement et de l'Environnement (https://edsmre.univ-lille.fr)

Funding: Global PhD Fund (KULeuven/ULille)

Laboratory: PC2A (CNRS/ULille) and CREaS (KULeuven)

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Duration and starting date: 4 years, starting from October 2024

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About PC2A

PC2A (Physico-Chimie des Processus de Combustion et de l'Atmosphère) is a joint laboratory of the CNRS and the University of Lille, in which transdisciplinary research has been performed for more than 60 years in the fields of combustion and atmospheric chemistry. Based on a strong interaction between experimental and modeling work, the researchers in PC2A crave at building better understanding of the science behind the challenges of the current society, such as clean and safe energy, and the mitigation of, and adaptation to climate change.

About CREaS

Our core activities are related to (bio)Chemical Reactor Engineering and Safety. We aim to innovate (bio)chemical reactor technologies for a few carefully selected and industrially relevant target areas. Our goal is to push the boundaries of our discipline and increase the performance and safety of (bio)chemical processes.

With the Department of Chemical Engineering, we aim to provide a balance between creative fundamental and applied research by integrating expertise, methodologies, and techniques from different domains in chemical engineering. These range from analyzing micro-to macroscopic process through modeling and design, optimization and control, and advanced experimentation. Given the prevalence and economical importance of the chemical process industry in Belgium, the societal role of our department in the education and training of the next generation of chemical engineers is very important.

At KU Leuven, we offer a competitive and international working environment with access to the latest technologies and expertise. At our university, we commit to create an inclusive, respectful, and safe environment. KU Leuven ranks among the top 10 universities in Europe (top 50 worldwide) in the major university rankings.