Towards the high-fidelity simulations of multicomponent sprays: multiscale modelling, numerical simulation and mathematical analysis

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Context

The search for low-carbon solutions, particularly for energy and transport, has led industry to devote a great deal of effort to hydrogen and synthetic liquid fuels, in order to reduce greenhouse gas emissions worldwide. Synthetic liquid fuels have the advantage of being similar to conventional fuels (calorific value, energy per mass or volume, distillation curve, etc.). On the other hand, their composition is very different. To optimize the combustion process or develop new combustor architectures, we need to understand and model the behavior of these synthetic fuels, particularly through numerical simulations.

As the composition of synthetic fuels differs from that of conventional fuels, droplet creation, turbulent transport and evaporation, crucial phenomena involved in combustion, can be widely modified and must be carefully determined. One of the most important aspects is the management of multi-component evaporation (MCE). Indeed, effects such as preferential evaporation of specific components or even dilution of the carrier gas in the fuel can radically alter the combustion process and, consequently, the efficiency of the whole system. The aim of this project is therefore to continue numerical developments in order to acquire a simulation tool capable of accounting for the physical phenomena involved in the evaporation of a drop formed from a multi-component mixture within a turbulent flow.

Objective of the post-doctoral position

In order to feed and develop evaporation models, which are often built from simplifying assumptions that turn out to be incorrect or imprecise, we wish to opt for the detailed simulation of droplet evaporation, predicting the flow into and out of the drop from fully coupled multifluid methods. Precursory work exists in the literature on this subject, and the thesis work of V. Boniou (EM2C) in particular clarified the methods to be employed and developed a solver (TITAN, available at EM2C) to solve such problems. However, this work has also confirmed a strong limitation of such simulations, notably linked to the treatment of jump conditions at the interface and to the precise description of species and temperature gradients, which determine mass and enthalpy fluxes at the interface. The aim of this project is to improve the numerical accuracy and efficiency of solvers for droplet evaporation. High-resolution methods, developed by the supervisors, will be studied and implemented in two aspects: interface representation and scalar resolution.

The candidate

This highly multidisciplinary project will require skills in physical modeling, numerical simulation, mathematical analysis, scientific computing and even high-performance computing.