DIPARTIMENTO DI INGEGNERIA
CORSO DI DOTTORATO IN INGEGNERIA INDUSTRIALE E DELL'INFORMAZIONE -
PHD COURSE IN INDUSTRIAL AND INFORMATION ENGINEERING -
34TH CYCLE

Title of the research activity:	Computational Fluid Dynamics (CFD) modeling of trans- and super-critical multicomponent flows
State of the art:	Trans- and supercritical conditions are often found in recent designs of direct injection engines, rocket engines and gas turbines for jet propulsion at take-off. More efficient and cleaner combustion technologies can be achieved increasing the operating pressure of the combustion chamber, leading to trans-critical trajectories of the injected liquid fuel [1-2]. Detailed understanding of real-fluid flows under these operating conditions is crucial [3-5]. With the increase of liquid bio- and synthetic fuels for aviation and transportation, further challenges are encountered in the engineering design of reliable and low-emission combustors. Recent computational studies have clearly shown the link between the injector flow and the mixing and auto-ignition occurring under these conditions [1,6], but numerical challenges and real-device complexities still pose challenges to full model predictivity. Despite its engineering importance, multi-component real-fluid spray in hot turbulent flows has not been explored thoroughly, yet and the scientific community lacks detailed understanding of the non-linear physics. The reason lies in the complex transitioning thermodynamics and in the multi-scale and multi-physic nature of the problem. At the realistic physical scale of combustion chambers, accurate description of the early phase of the dense spray break-up and atomization for multi-component fuels is especially important, but first-principle prediction of such complex phenomena is a challenging task. Two main classes of Eulerian methods exist. On one hand, sharp interface methods, like level-set (LS) and volume-of-fluid (VOF) methods, can be used in the subcritical regime for directly resolving the interface mechanics [12-14], but these methods are computationally demanding as the interface features may be extremely small. On the other hand, diffuse-interface models, based on two-fluid or single-fluid formulations [1-7,15,16], are less computational demanding and can be applied to large scale spray or combustion chamber design, but research is needed for accurate closure models of sub-grid effects. Our recent work has already investigated the possibility of introducing real-fluid properties in to single-fluid Eulerian models [7,10,13]. In this PhD project, in order to enhance the prediction capabilities in high-pressure high-temperature multi-component two-phase regions, we plan to explore and compare multiple paths, by developing new solvers in OpenFOAM for: - Single-fluid model description, - Two-fluid model, where two phases are directly transported, with the addition of a transport equation for the interfacial area density, which will allow to calculate the local level of atomization, like droplet/ligament size, and which will vanish at supercritical condition [8-11,17]. Each approach will combine real-fluid thermodynamics properties. These models can be naturally and seamlessly coupled to already exiting combustion models, then enabling the unified simulation of two-phase and reactive flow cases. These approaches represent the first attempt in the literature to couple the surface area density with the flow variables, in the context of real-fluid thermophysical models.

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<tr><td></td><td>Ultimately, these solvers will be applied to the study of novel fuel injection conditions, novel high-efficiency engines, and renewable e-fuel injection and combustion.</td></tr>
<tr><td>Short description and objectives of the research activity:</td><td>The research aims to develop a new two-phase flow solvers for fuel sprays with specific focus on high pressure and high temperature conditions, and multicomponent thermodynamics. The code will be developed in OpenFOAM and will be able to describe in Eulerian form the processes of primary atomization and mixing in subcritical and supercritical conditions.

The project is within the area of CFD Modeling of Fuel Sprays and Combustion. The candidate is expected to have good knowledge of
- CFD modeling and numerics,
- C/C++ programming,
- python/matlab scripting is a plus.
The successful candidate will perform large-eddy simulations (LES) of two-phase flows using high-performance computing (HPC) resources; he will also incorporate state-of-the-art experimental measurements to improve the accuracy of the models. Eventually, the candidate will write peer-reviewed journal articles, and present the results of the work at international conferences and events.</td></tr>
<tr><td>Bibliography:</td><td>1. Chung W. T., Ma, P. C., Ihme, M., "Examination of diesel spray combustion in supercritical ambient fluid using large-eddy simulations." International J of Engine Research, 2020, 21:1, 122-133.
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