

**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:	Predictive Models and Experimental Validation of Multicomponent Dense Spray Dynamics
State of the art:	<p>The topic is related to the strong interest towards new combustion concepts and emission reduction in transportation and power generation sectors. 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 [1]. First, as in DNS, the level-set (LS) and volume-of-fluid (VOF) methods in the subcritical regime may be used for directly resolving the interface mechanics [2,3], but these methods are computationally demanding as the interface features may be extremely small. For applications with fine-scale atomization regimes, an alternative approach is to use a generalized two-phase flow formalism based on the concept of inter-penetrating continua. Two-fluid or single-fluid (mixture) models can be formulated [1,4,5,6]. These Eulerian methods do not track the interface, and result in a diffuse-interface modeling approach. These approaches offer the advantages of natural inclusion of the energy equation, with complex equation of states for the fluids, phase change and compressibility, however, further research is needed for accurate closure models of sub-grid dispersion [7]. In addition to the above aspects concerning the mechanics of spray atomization, another extremely relevant topic is the effect of multi-component liquids on the dynamics of dense sprays in an Eulerian frame of reference. To our knowledge, no modeling framework existent today can adequately address this issue. Multi-component liquids undergoing phase change exhibit preferential evaporation of some species with respect to others [8]. This creates complex gas mixture environments which drastically affect the subsequent combustion.</p>
Short description and objectives of the research activity:	<p>The research aims to develop a new two-phase flow solver 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.</p> <p>The project is within the area of CFD Modeling of Fuel Sprays and Combustion. The successful candidate will collaborate with EU and extra-EU university partner groups. The 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.</p>
Bibliography:	<ol style="list-style-type: none"> 1. Gorokhovski, M., & Herrmann, M. (2008). Modeling primary atomization. <i>Annual Review of Fluid Mechanics</i>, 40(1), 343-366. 2. Vukcevic, V., Jasak, H., Gatin, I. (2017). Implementation of the ghost fluid method for free surface flows in polyhedral finite volume framework. <i>Comput. Fluids</i>, 153, 1-19. 3. Tomar, G., Fuster, D., Zaleski, S., & Popinet, S. (2010). Multiscale simulations of primary atomization. <i>Computers & Fluids</i>, 39(10), 1864-1874. 4. Xue Q., Battistoni M., Powell C.F., Longman D.E., Quan S.P., Pomraning E., Senecal P.K., Schmidt D.P., Som S. (2015). An Eulerian CFD model and X-ray radiography for coupled nozzle flow and spray in internal combustion engines. <i>Int. J. of Multiphase Flow</i>, 70, p. 77-88. 5. Battistoni M., Xue Q., Som S. (2016). Large-Eddy Simulation (LES) of Spray Transients: Start and End of Injection Phenomena. <i>Oil & Gas Sc. and Tech.</i>, 71.

	<p>6. Matheis J., Hickel S., (2018) Multi-component vapor-liquid equilibrium model for LES of high-pressure fuel injection and application to ECN Spray A, <i>Int. J. of Multiphase Flow</i>, 99, p. 294-311.</p> <p>7. Demoulin, F., Reveillon, J., Duret, B., Bouali, Z., Desjonqueres, P., Menard, T. (2013). Toward using direct numerical simulation to improve primary break-up modeling. <i>Atomization and Sprays</i>, 23(11), 957-980.</p> <p>8. Sazhin, S. S. (2006). Advanced models of fuel droplet heating and evaporation. <i>Progress in Energy and Combustion Science</i>, 32(2), 162-214.</p>
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