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# The role of detailed chemical kinetics on CFD diesel spray ignition and combustion modelling

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ABSTRACT

Spray ignition and flame stabilisation in the frame of diesel-like combustion conditions combine fundamental and complex physical and chemical processes. In this work, a numerical investigation has been performed to evaluate the potential of integrating detailed chemistry into CFD calculations, in order to improve predictions and gain more insight in involved processes. This work has been carried out using the capabilities of OpenFOAM©code, which provides an opensource framework for 3D-CFD simulations, including an ODE solver for solving chemical kinetics. As a general methodology, this study is based on simulating free *n*-heptane sprays injected into a constant volume vessel, corresponding to the conditions of the experimental database provided by Sandia National Laboratories. Calculations results have been compared to experiments, evaluating the effect of a wide range of ambient conditions on spray ignition and combustion characteristics. Specifically, this research checks the performance of some relevant *n*-heptane oxidation mechanisms found in the literature, with different degree of complexity, for modelling the chemical history of the fuel. The results of this investigation show the relative influence of chemical mechanism on spray/flame structure in terms of ignition delay and also ignition and flame stabilisation sites. The comprehensive mechanism performs generally better than more simplified chemistry models. However, its accuracy is also compromised for modelling advanced diesel-like combustion concepts based on injecting the spray into a low oxygen concentration environment.



## 1. Introduction

Nowadays, turbulent combustion modelling represents an extremely complex, but also an important, challenge for the research community due to its undoubtable technological interest. According to Veynante and Vervisch [1], computing is now truly on a par with experiment and theory as a research tool to produce multi-scale information that is not available by using any other technique. In the last decade, computational fluid dynamics (CFD) is being extensively used to design a wide range of combustion systems and then, much work has been devoted to turbulent combustion modelling.

These authors identify a wide range of coupled problems involved in turbulent flames. Among other aspects, the fluid mechanical properties of the combustion system must be well-known to carefully describe all transfer phenomena occurring in turbulent flames and detailed chemical reaction schemes are necessary to estimate the consumption rate of the fuel, the formation of combustion products and pollutant species. Additionally, a precise knowledge of the chemistry is absolutely required to predict ignition, stabilisation or extinction of reaction zones together with pollutant formation. Consequently, the key role of the performance of chemical kinetic mechanisms for producing accurate results in the frame of CFD turbulent combustion modelling is evident.

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