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Simulation of reacting flows using artificial neural networks: application to multi-regime combustion

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The simulation of reactive flows is a major challenge in several industrial sectors, such as aeronautics or energy production. The coupling between fluid dynamics and chemistry comes however at a cost, as chemical processes involve a wide range of spatial and time scales. The resulting equations are stiff and require specific, and expensive, numerical methods. A strategy often adopted in the past decades to circumvent this issue is to tabulate the chemistry [1]. In such methodologies, the chemical processes are computed in a pre-processing step and reactions rates are retrieved from a table during the actual simulations. Nevertheless, reaction rates must be accessed in the table using a reduced set of coordinates. It is therefore not adapted to complex combustion systems for which chemical trajectories evolve on complex manifolds.

More recently, several teams have proposed the use of machine learning to estimate the reaction rates. In particular, Artificial Neural Networks (ANN) have the capability to make interpolation on high-dimensional data and are thus particularly adapted to chemistry problems [2,3]. A major issue is then to select an appropriate database on which to train the ANN. It must: (i) be representative of the targeted application; (ii) be sufficiently quick to generate. A promising strategy is to use 0D stochastics reactors [4], which mimic reactive and mixing processes in systems while being relatively cheap to compute. This methodology has been successfully applied to diffusion flames [4]. In the present work, the aim is to show the ability of the 0D stochastic reactors to be used as a database for complex combustion system. In particular the focus will be on the ability to predict multi-regime combustion, where both premixed and diffusion burning modes take place.

In this study, we first propose a methodology to generate a database for multi-regime combustion using 0D stochastic reactors. An ANN is then trained on the data and validated on the following simulations: (i) purely premixed flames; (ii) pure diffusion flames; (iii) a triple flame configuration involving both diffusion and premixed combustion modes. The generated network is shown to reproduce these combustion regimes with good accuracy in *a priori* and *a posteriori* tests. The obtained results pave the way to the application of ANN coupled to 0D stochastic reactors databases to industrial cases.

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