Modeling the chemical structure of spray flames using tabulated chemistry method

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Abstract

A complete comprehension of the spray combustion is necessary to guarantee security and to reduce pollutant emissions in aircraft combustions and internal combustion engines. Spray combustion presents a complex nature, comprising liquid dispersion into droplets and evaporation, and is an active topic of research. The fuel droplets evaporation process causes strong inhomogeneities of equivalence ratio in the fresh gases. The chemical structure of the spray flame is therefore highly complex presenting premixed-like and non-premixed-like reaction zones. Numerical prediction of the combustion phenomena such as the flame propagation or the pollutant predictions, which are particularly sensitive to detailed chemical effects, is very challenging and requires a precise and reliable chemical description. Flamelet-based tabulated chemistry methods have been initially developed to introduce detailed chemistry in gaseous flames with a reasonable computational cost. They assume that the local turbulent flame structure is similar to those of single flamelet elements. For instance, PFT methods are based on fully-premixed flamelets whereas the DFT tables are constructed using diffusion flamelets. These approaches seem to be unable to predict the complex chemical structure of spray flames since they are based on a single combustion regime. Multi-regime flamelet methods have recently been proposed to model the structure of complex flames where both premixed-like and diffusion-like reactive layers are present and seem better adapted for spray flames. The performance of tabulated chemistry method for spray combustion is attractive but it has never been rigorously identified. The present work analyses the capability of tabulated chemistry methods to model the chemical structure of spray flames assuming that the chemical subspace accessed by a spray flame can be mapped by a collection of adiabatic gaseous flamelets. Different tabulated chemistry strategies are considered: the PFT method, based on premixed flamelets, the DFT approach, based on diffusion flame elements, and a new technique called Partially-Premixed Tabulated Flamelet (2PFT). In the 2PFT method information from partially-premixed flames are stored into a 3-D look-up table parametrized as function of the progress variable Y_c, evolving monotonically between fresh and burnt gases, of the mixture fraction Y_z, denoting the local equivalence ratio, and the scalar dissipation rate of the mixture fraction χ^*, which identifies the combustion regime.

The three techniques have been tested on a 1-D laminar axisymmetric counterflow kerosene/air spray flame. Since the spray flame structure strongly depends on the gas and liquid phase properties at injection, an exhaustive collection of spray flames has been calculated using a detailed kinetic mechanism and complex thermodynamic properties, for different values of the liquid and gas velocity, the droplet diameter, the liquid volume fraction and the injection temperature at injection. The capability of the PFT, DFT and 2PFT techniques to reproduce the structure for all the considered spray flames has been assessed and the impact of mapping spray flames with a chemical subspace on adiabatic and gaseous flamelets has been evaluated.

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