A MULTI-REGIME FLAMELET METHOD FOR PREMIXED AND NON-PREMIXED COMBUSTION IN SPRAY FLAMES

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Summary Tabulated chemistry is an attractive technique to account for detailed chemical effects with an affordable computational cost but its performances for spray combustion have never been identified. In this work, we will discuss the chemical structure modeling of spray flames using tabulated chemistry methods under the hypothesis that the chemical subspace accessed by a two-phase reactive flow can be mapped by a collection of gaseous and adiabatic flamelets. A new multi-regime flamelet tabulation method (TPPC) will be presented and will be tested on counterflow laminar spray flames for different injection conditions. Results will be compared to detailed chemistry calculations and to the classical FPI and FPV tabulation methods.

Introduction

Predicting the flame structure and the pollutant formation of spray combustion requires careful description and comprehension of the chemical phenomena. Tabulated chemistry is a popular technique to account for detailed chemical effects with a reasonable computational cost [1]. This approach is based on the idea that the turbulent flame structure is similar to those of single flamelets elements representative of a single burning regime. Then, the composition space accessed by the turbulent flame can be parametrized and tabulated by a reduced subspace, decreasing the computational cost. Although tabulated chemistry is an attractive technique, its capability to reproduce spray flames has never been evaluated. In the following, we will present an enhanced tabulated chemistry method called Tabulation Partially Premixed Combustion (TTPC) that increases the range of validity of the model by adding a coordinate related to the mixture fraction scalar dissipation rate to the chemical look-up table. The impact of mapping spray flames with a tabulated chemistry on adiabatic and gaseous flamelets is finally evaluated on counterflow spray flames.

The new TPPC method

Among the different strategies to generate chemical look-up tables, some of them are based on physical considerations like the FPI [2] or the FPV [3] method. In these techniques, a 2-D (Y_c,Y_z) subspace is generally built from laminar premixed or diffusion flamelets respectively. Y_c is the progress variable, evolving monotonically between fresh and burnt gases, and Y_z is the mixture fraction, representing the local mixture equivalence ratio. However, as demonstrated in [4, 5], for partially-premixed flames the effective dimension of the accessed composition space is higher because of the fluxes across iso-equivalence-ratio and iso-progress-of-reaction surfaces. In such situations, supplementary coordinates such as the scalar dissipation rate for the mixture fraction and/or for the progress variable should be added.

In the new TTPC method, a collection of 1-D gaseous partially-premixed counterflow flamelets formed by a fuel/air mixture injected against air is calculated for different values of the strain rate $0 < a < a^{ext}$, where a^{ext} is the extinction limit. The fuel/air stream (superscript f) equivalence ratio ϕ^f is also varied between $\phi^f = \phi^f_L$ and $\phi^f = +\infty$, where ϕ^f_L is the smallest value of the fuel/air stream equivalence ratio for which a counterflow flame is stabilized at a given strain rate. The subspace accessed by both premixed and non-premixed flames is identified by three parameters: the progress variable Y_c, the mixture fraction Y_z and $\chi^* = |\nabla Y_z|^2$ which is linked to the scalar dissipation rate of Y_z. For each point (Y_c,Y_z,χ^*) covered by the database there is only one corresponding flamelet and any thermo-chemical quantity φ is then obtained from the 3-D look-up table:

$$\varphi = \varphi[Y_c, Y_z, \chi^*]. \tag{1}$$

The additional parameter χ^* covers the composition subspace between premixed ($\chi^* = 0$) and diffusion flamelets passing through partially-premixed flames, the maximum value of χ^* corresponding to diffusion flames. The TPPC method solves the flame in the physical space and does not require any modeling of χ^* unlike methods proposed in [4] or [5] where the flame structure is resolved in the composition space.

Results

In a counterflow mono-disperse spray flame (Fig. 1a), pure air is injected on the left side against liquid fuel and pure air injected from the right side (superscript f). Its structure strongly depends on the gaseous flow properties as well as the characteristics of the spray, such as the droplet diameter D_l, the liquid temperature T_l, the liquid volume fraction α_l and the density droplet number n_l. The capability of the TPPC tabulation method to capture the structure of a kerosene spray flame has been investigated for different injection parameters values but in the following only one representative case is discussed: $D^f_l = 40\ \mu m$, $\alpha^f_l = 3.0\ 10^{-3}$, gas and liquid injection velocity $v^f_g = v^f_l = 0.20\ m/s$ and gas and liquid temperature $T^f_g = T^f_l = 400\ K$.

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The TPPC look-up table is based on the progress variable $Y_c = Y_{CO} + Y_{CO_2}$ [6], on the quantity χ^* and on the mixture fraction Y_z:

$$Y_z = \sum_{k=1}^{N_{spec}} n_{Ck} \frac{Y_k W_C}{W_k}, \tag{2}$$

with W_C the element weight of carbon, N_{spec} the number of species of the reference detailed chemistry, and n_{Ck} and W_k the number of carbon atoms and the molecular weight for the k^{th} species, respectively. The table is composed by a collection of adiabatic gaseous counterflow flames for ten different values of ϕ^f and for different values of the injection velocity $v_g^{ox} = v_g^f$ comprised between $0.2\ m/s$ and $10\ m/s$. All these flames have been calculated imposing the injection temperature of the spray flames equal to $400\ K$. Heat losses are neglected when building the database but we have checked that the adiabaticity assumption is reasonable for the studied cases.

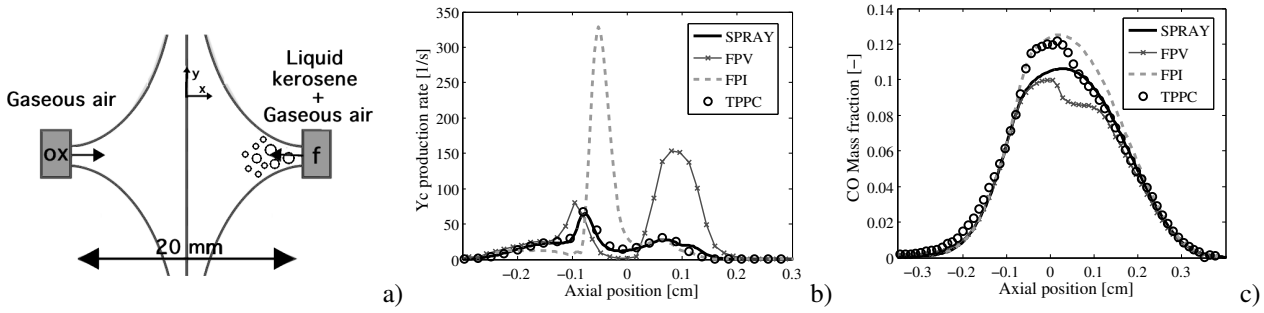

Figure 1. a) The counterflow configuration. b) Production rate of the progress variable $\dot{\omega}_{Y_c}$ and c) CO mass fraction for the reference spray flame. Black continous line: detailed chemistry. Dashed gray line: FPI premixed database. Gray crosses: FPV diffusion method. Black circles: TPPC technique.

All spray and gaseous flames have been simulated with the REGATH-counterflow code [7] using a detailed mechanism for kerosene/air flame comprising $N_{spec} = 91$ species and $N_{reac} = 991$ reactions [8]. To simplify the calculation kerosene is represented by the $C_{10}H_{22}$ species and unity Lewis number is assumed for all species.

The production rate of the progress variable $\dot{\omega}_{Y_c}$ (in $1/s$) for the spray counterflow flame is plotted in Fig. 1b (continuos black line). From reference values of Y_c, Y_z and χ^*, the quantity $\dot{\omega}_{Y_c}$ is extracted from FPI (dashed gray line), FPV (gray cross symbols) and TPPC (black circles) look-up tables respectively. A first premixed-like region is found in the zone near the evaporation where a very rich mixture is obtained due to evaporation ($0.1\ cm < x < 0.2\ cm$). The FPV method overestimates $\dot{\omega}_{Y_c}$ in this zone whereas the FPI method seems to offer more accurate results. A non-premixed-like reaction zone could be observed for $-0.25\ cm < x < -0.1\ cm$ where intermediate species and products are mixed and recombined with the fresh air coming from the left injection. In this region, the FPV method is more adequate compared to FPI. The TPPC methodology is able to accurately describe the production rate in the whole reaction region characterized by both premixed and non-premixed combustion regimes. The CO mass fraction is represented in Fig. 1c with the classical methods and the TPPC formulation. As already observed for the production rate $\dot{\omega}_{Y_c}$, only the TPPC method accurately reproduces the whole flame structure. This behavior has been observed in all studied cases: the TPPC tabulation method correctly describes the structure of the spray flames which are characterized by different combustion regimes.

Conclusions

A new chemical TPPC tabulated chemistry has been presented based on the progress variable Y_c, the mixture fraction Y_z and χ^*. Three tabulation methods (FPI, FPV and TPPC) have been analyzed on spray flames for different injection parameters values. In all tested cases, the TPPC tabulation method better describes the flame structure compared to the classical techniques based on a single archetypal flamelets and it is more adequate for counterflow spray flames. It has been demonstrated that the chemical structure of laminar spray flames could be modeled by a tabulated multi-regime flamelet combustion regime based on gaseous flamelets.

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