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Numerical investigation of soot-flame-vortex interaction

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Abstract

Because the numerical simulation of soot production in turbulent flames is quite challenging, it is useful to consider simpler aerodynamic configurations retaining unsteady strain rate and curvature effects. The present article reports detailed numerical simulations of a planar vortex interacting with a sooting laminar diffusion flame formed by a parallel flow of acetylene and air. Calculations are carried out to reproduce the experimental data reported by Cetegen and Basu (2006). Compared to previous numerical works on this configuration based on simple two-equations soot models, a detailed numerical mechanism, accounting for 97 gaseous species and 59 solid BINs, is considered here to represent the chemistry in the gas phase and the production and oxidation of soot particles. Three different vortex strengths are considered and vortices are formed by pulsing the air or the fuel streams, allowing comparisons between the calculated soot-vortex-flame interactions with LII images. Calculations adequately retrieve experimental data when the vortex is initiated at the fuel side. Differences are observed when the vortex is formed on the air side. The simulations, however, are useful for examining strain rate and curvature effects on soot volume fractions of small spherical particles and large aggregates, and to study physical processes underlying the soot production. It is shown that the variability of the soot volume fraction is highly correlated to the response of soot precursors to flame curvature. Soot variability in the mixture fraction space depends on the behavior of large aggregates that, being characterized by high Schmidt numbers, are more sensitive to the convective motion imposed by the vortex compared to the gaseous phase. The observed behavior has to be reproduced by the models developed for numerical simulations in order to obtain an accurate prediction of soot production in turbulent flames.

Keywords: Soot; Curvature; Vortex; Strain rate; Heavy PAHs

1. Introduction

Reducing soot emissions is of considerable importance for many practical applications due to their negative effects on the environment and on public health. In this context, substantial experimental and numerical efforts have been made to

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understand, characterize, and model the complex processes leading to soot formation and oxidation [1–4].

Soot production[1] in turbulent flames, which are most relevant in practice, is a complex process which depends on chemistry, flow history and local turbulence properties. The analysis of soot in fully turbulent flames is then extremely challenging. The experimental investigation requires the use of combined diagnostics to obtain quantitative measurements of soot distribution, its relation with respect to flow and flame quantities [5–8]. On the numerical level, Direct Numerical Simulations (DNS) of turbulent flames have been used to investigate the dependence of soot production on the flow history and local turbulence properties [9–16].

Alternatively, simpler configurations may be used to study flame-flow-soot interactions for a reduced computational cost. This is exemplified in the cases of a laminar pulsed flame [17] or a diffusion flame wrapped-up by a line vortex [5]. In these two cases, measurements are more easily carried out than in fully turbulent flames because the phenomenon can be periodically reproduced. From a numerical standpoint, these configurations are attractive because they can be simulated using detailed models so that complex processes underlying soot production can be accurately described. Obviously, these fundamental studies do not replace the need for fully-turbulent simulations, but provide crucial information on the instantaneous and local effect of a vortex eddy on soot production that could be used to clarify the turbulent flame behavior and to guide the modeling efforts.

The flame-vortex interaction is specifically useful and has been extensively explored to investigate the effects of unsteady strain rate and curvature induced by vortices on the flame front [18]. Among various generic configurations, the case of a planar diffusion flame wrapped-up by a line vortex is considered in the present investigation and simulated with a detailed model for gas dynamics and soot particle production that cannot be afforded in DNS of turbulent flames. Using an elegant experimental design, Cetegen and Basu [5] were able to obtain soot volume fraction distributions from LII imaging. Previous numerical studies of this configuration [19,20] have used simplified gaseous mechanisms and soot models based on semi-empirical two-equation representations, with a limited degree of generality. In the present work, we propose a detailed numerical simulation of soot-flame-vortex interaction based on a detailed description of both gas and soot, together with a direct comparison between experiments and simulations on the effect of vortices on soot production.

[1] Soot production indicates the net process comprising both formation and consumption contributions.

Calculations are carried out to examine effects related to the injection side and to the vortex strength. The paper begins with a review of the detailed kinetic mechanism (Section 2). The numerical setup is briefly presented in Section 3. The interaction of a vortex with soot is analyzed in Section 4. The analysis focuses on the influence of curvature on the flame quantities governing soot production and on the effect of the flow field induced by the vortex on the soot layer.

2. Detailed kinetic mechanism

The kinetic scheme combines a detailed gas-phase mechanism (DGM) and a detailed soot mechanism (DSM) for the description of the formation and oxidation of soot.

The DGM consists of $\sim$ 170 species and $\sim$ 6000 reactions, describing the high-temperature pyrolysis and oxidation for a wide range of hydrocarbon fuels [21]. The mechanism has been tested over a wide range of conditions [22,23].

The DSM was developed using the discrete sectional method [24]. Only the most relevant details are provided in what follows. PAHs (Polycyclic aromatic hydrocarbons considered soot precursors) are organized in two classes: light PAHs, including species up to pyrene, and heavy PAHs, including species with more than 4 aromatic rings. Heavy PAHs and particles are discretized into 20 classes of pseudo-species (called BINs) with their masses doubled from one class to the next. PAHs of more than 20 carbon atoms constitute the first four BINs. The first soot particles (BIN5) are modeled as clusters containing 320 carbon atoms. Particles between BIN5 and BIN12 are assumed to be spherical in shape with a mass density of 1500 kg m^{-3} [25]. BIN13 to BIN20 are treated as monodisperse aggregates, with fractal dimension of 1.8 [26]. The DSM features a total number of 100 lumped pseudo-species organized in 20 BINs, each of which has two or three subclasses (different H/C ratios), split into radical or molecular surfaces. Six heterogeneous reaction classes are accounted for with appropriate kinetic parameters: hydrogen-abstraction-carbon-addition (HACA) mechanism; inception; oxidation; surface growth; dehydrogenation; coalescence and aggregation. The total number of reactions for the DSM scheme is $\sim$ 10500.

To enable computational simulations, the mechanism was reduced with the Species-Targeted Sensitivity Analysis (STSA) technique [27]. The final mechanism, provided in the Supplementary material, includes 156 species (97 gaseous species and 59 BINs) and $\sim$ 5600 reactions. Species transport properties are calculated from the standard molecular theory of gases. Soot particles and aggregates are treated as gaseous species, so that their binary mass diffusion coefficients are calculated on the basis of a proper extrapolation from the binary mass