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Unsteady dynamics of PAH and soot particles in laminar counterflow diffusion flames

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Abstract

Due to their low chemical time scales, the production of soot particles in turbulent diffusion flames is highly impacted by large range of local strain rate fluctuations.

In order to understand the response of soot production to strain rate fluctuations, unsteady laminar counterflow diffusion flames with an imposed oscillating strain rate are investigated both analytically and numerically. First an analytical linearized model is developed to predict the unsteady response of a flame quantity of interest from information on laminar steady flames. Three critical parameters governing flame response are identified: the Stokes number which compares the characteristic time associated to the mean imposed strain rate to the oscillation frequency, the Damköhler number associated to the quantity of interest, and a third one characterizing the response of this quantity to an imposed steady strain rate. This model is then applied to soot predictions. Parallely, the response of soot production in propane-air counterflow diffusion flames to unsteady strain harmonic oscillations is studied numerically using a detailed sectional soot model. A wide range of frequencies and amplitudes are considered. A specific trend is highlighted for soot precursors and particles production according to their respective chemical time scales: the bigger the PAH or soot particle, the higher its chemical time scale, resulting in a more damped and phase-lagged response. The particle size distribution evolves accordingly during the considered oscillations, so that the quasi-steady state behavior is not verified for high frequencies. The numerical results are compared to those obtained by the analytical approach and a very good agreement is obtained at low amplitudes. Non-linear response of soot precursors and soot particles production to strain oscillations are finally discussed in case of high oscillation amplitudes and the limits of the proposed analytical model are identified.

Keywords: PAH; Laminar flame dynamics; Soot sectional model; Particle size distribution; Unsteady strain rate

1. Introduction

Due to incomplete combustion, soot emissions have effects on both human health and environment. Soot emissions are also considered as an

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important cause of global warming [1]. Consequently, important efforts are made both experimentally and numerically [2–4] to understand soot production mechanisms in order to control their emission.

Most of the combustion facilities are characterized by high Reynolds number flames where turbulent eddies are expected. The local strain rate usually fluctuates in a wide amplitude range and with random fluctuation frequencies [5]. These turbulent eddies are also responsible for variable length scale recirculation zones, introducing a wide range of residence times for soot particles, strong intermittency and dynamics features in soot production [6,7].

One of the most popular approaches used to simulate turbulent non-premixed flames is the flamelet approach, based on a quasi-steady response of the flame characteristics to the local strain rate fluctuations [8,9].

The development of such models being motivated by the application to numerical simulations of turbulent flames, the response of soot to strain rate fluctuations can be investigated by looking at unsteady laminar counterflow diffusion flames [10–12]. Specifically to soot context, previous experimental works have been performed in a diffusion laminar flame by introducing sinusoidal velocity variations at both opposed nozzles [13,14]. They showed that soot production response to these fluctuations was phase-lagged and damped when increasing the oscillation frequency. A particular hierarchical behavior was observed: soot volume fraction response is more phase-lagged and damped compared to soot precursors response, which are also more phase-lagged and damped than the temperature response [15]. Cuoci et al. [17] numerically investigated these flames with good prediction of unsteadiness soot dynamics, confirming the experimental observations. Nevertheless, a lack of knowledge remained on the origin of soot response to unsteady strain fluctuations. Moreover, when computing counterflow diffusion flames with unsteady velocities at the nozzle exits, a phase lag exists between the global strain rate and the local strain rate [17], increasing the complexity of the phenomena. In the other hand, other studies [16] also studied the transient behavior of PAHs production by studying their response to one-step variation of the strain rate. The objective was to derive tabulation methods relative to PAHs in a turbulent combustion modeling context, but no specific study of the soot particles hierarchical response to unsteady fluctuations completed these works.

The objective of the present work is to characterize the response of soot to strain rate oscillations and to identify the physical phenomena underlying the phase lag and damping observed in soot production. In order to avoid the phase lag between the global and the local strain rate, a strain-imposed formulation is considered in this work and unsteadiness is introduced by varying the imposed flame strain rate $a(t)$ with time for a given pulsation ω, an initial strain rate A_0 and fluctuation amplitude αA_0:

$$a(t) = A_0 + \alpha A_0 sin(\omega t) = A_0[1 + \alpha sin(2\pi f t)]. \quad (1)$$

Both analytical and numerical approaches are considered in this paper to study the evolution of the soot precursors and of the particle size distribution (PSD) with the strain rate $a(t)$.

The paper is organized as follows. First, an analytical model is proposed in Section 2 in the limit of a linear behavior, i.e. small oscillation amplitudes. This model predicts the unsteady response on the basis of steady flame results. Then, soot production in unsteady laminar flames is numerically studied using a detailed sectional model. The modeling strategy is introduced in Section 3. The flame response is then investigated for the configuration described in Section 4.1. The unsteady behavior is analyzed in Section 4.2 for different frequencies at small amplitude in terms of global quantities and PSD. Analytical results will be compared to the numerical ones in Section 4.3 to prove their validity. The causes of phase lag and damping in soot production will then be identified by combining information from numerical and analytical results. Finally, numerical simulations at high amplitudes are analyzed in Section 4.4 to completely characterize the soot response to unsteady strain rate oscillations and to discuss the limits of the analytical model.

2. Analytical model for pulsed sooting flames

In order to investigate the response of soot production to strain rate fluctuations, a linearized analytical model is developed in the following to predict the response of the maximum of a flame variable θ to strain rate oscillations at a given pulsation ω. The complex form of the fluctuating strain rate $a_1(t) = a(t) - A_0$ is denoted by $\hat{a}_1(\omega) = \alpha A_0 e^{j(\omega t - \pi/2)}$. The corresponding response of the maximum value of θ, namely $\theta^{max}(t) = \theta_0^{max} + \theta_1^{max}(t)$ with $\theta_1^{max}(t) = \theta_1^{max}(\omega) sin(\omega t - \varphi_{\theta^{max}}(\omega))$, is represented by the complex number $\hat{\theta}_1^{max}(\omega) = \theta_1^{max}(\omega) e^{j(\omega t - \pi/2 - \varphi_{\theta^{max}}(\omega))}$. This response is fully characterized by the transfer function $T_{\theta^{max}}(\omega) = \hat{\theta}_1^{max}(\omega)/\hat{a}_1(\omega)$.

Starting from the previous works [10–12], the transfer function is split into two terms: the transfer function $T_{unst}^{finite,\theta}(\omega)$, introducing an equivalent steady strain rate A_θ seen by the quantity θ, and the transfer function $T_{steady}^{\theta^{max}|A_\theta}(\omega)$, describing the response of θ^{max} to the equivalent steady strain rate A_θ.

2.1. Equivalent steady strain rate

Following [10–12], under the assumption of infinitely fast chemistry, the unsteady flame acts at