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Coupling an LES approach and a soot sectional model for the study of sooting turbulent non-premixed flames

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ABSTRACT

Due to their negative impacts on environment and human health, future regulations on soot emissions are expected to become stricter, in particular by controlling the size of the emitted particles. Therefore, the development of precise and sophisticated models describing the soot production, such as sectional methods, is an urgent scientific and industrial challenge. In this context, the first objective of this work is to use for the first time a sectional model to perform an LES of a sooting turbulent flames in order to demonstrate its capacities. For this, the whole LES formalism for this approach is developed. It includes state-of-art models for the description of the gaseous phase and an extension of a soot subgrid intermittency model to the sectional approach, originally proposed for the hybrid method of moments. Then, the LES is used to analyze a turbulent non-premixed ethylene–air jet diffusion flame and results are validated by available experimental data. The quality of results for the gaseous phase is satisfactory and results for the solid phase show a reasonable agreement with the experimental results in terms of localization, intermittency and soot volume fraction magnitude. Once the coupled LES-sectional approach validated, having access to the full information on the spatial and temporal evolution of the soot Particle Size Distribution (PSD), the second objective of this work is to provide a new fundamental insight on soot production in turbulent non-premixed flames. First, it is observed that a one-peak and a two-peak PSD shapes are observed at the bottom and downstream of the flame, respectively. Second, high fluctuations of the PSD distribution is observed all along the flame. In particular, a time bimodal behavior is observed with the presence of a zone with regular transitions between one- and two-peak PSD shapes. By analyzing soot particles Lagrangian paths, these high fluctuations are shown to be linked with the wide range of history paths of soot particles, which are mainly driven by turbulence.

1. Introduction

Soot particles result from an incomplete combustion of hydrocarbon fuels and are generally undesirable due to their harmful impacts on both environment [1] and human health [2].

The prediction of soot emission is extremely challenging due to its complex nature, characterized by a strong coupling between flow parameters, flame characteristics and soot properties. This is even more difficult when studying soot production in turbulent flames, where the chemical scales underlying soot production compete with the turbulence scales [3–5].

Therefore, the numerical prediction of soot requires adequate and precise models for the characterization of the turbulent behavior of the flame as well of the different phenomena involved in soot production. Different strategies have been proposed in literature as a compromise between accuracy and computational cost. On the one side, Direct Numerical Simulations (DNS), providing a full description of all the temporal and spatial scales, and Large Eddy Simulations (LES), resolving only the most energetic scales, have been used to investigate turbulent soot production in academic configurations [5–7] or more realistic flames [8–12], respectively. However, due to their high computational cost, these simulations rely on simplified description for the soot evolution, i.e. semi-empirical models [13,14,24] or methods of moments [15–18], which usually do not provide access to the soot particle size distribution (PSD). Therefore, these approaches allow an adequate description of the spatial and temporal evolution of the flow and the flame, but not of the soot PSD. Nevertheless, method of moments can provide an accurate description of soot fractality at a low cost, by using bi-variate moments of the soot PSD in particles surface and volume spaces [16,21,23]. On the other side, due to their high computational cost, the use of sectional methods, a discretized representation of the soot par-

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ticle size distribution in the particles volume space, have been limited to Reynolds Averages Navier Stokes (RANS) computations [26–28]. This RANS-sectional approach provides access to more details in soot particle size distribution spatial evolution while losing information on the flow and the flame, for which only ensemble-average statistics are available.

In this work, we propose to exploit the whole potential of both strategies, by combining an LES approach with a sectional model for the prediction of soot particles evolution, in order to access new information about soot particles dynamics in turbulent flames through the study of their particle size distributions. To our knowledge, this approach has never been tackled until now.

In this context, the objective of this paper is twofold. First, the feasibility and validity of LES approach based on a sectional model are demonstrated for sooting turbulent non-premixed flames. For this, the soot sectional model is reminded in Section 2. Then, the LES formalism is introduced in Section 3, by presenting the models for all the unclosed terms of the filtered equations for the solid phase description. In particular, the soot intermittency subgrid model developed in [29] for the hybrid method of moments is extended to the soot sectional model. The model is then applied in Section 4 to the simulation of an ethylene/air jet diffusion flame. Temperature and species radial profiles are compared to experiments. Concerning soot particles evolution, axial and radial profiles of mean and root mean square (RMS) of soot volume fraction are compared to experiments.

Once the LES approach validated and having access to the full information on soot production phenomena, the second objective of this work is to investigate soot production in turbulent flames. Soot formation is then analyzed in Section 5 through the study of the different source terms involved in soot production. The major contributors of soot production are then identified. Thanks to the coupled LES-sectional approach, information on the spatial and temporal evolution of the PSD are numerically accessible for the first time, whereas only evolutions about the moments of soot PSD were previously analyzed thanks to the method of moments [22,25]. In the current study, high fluctuations between one-peak and two-peak PSD shapes are observed along the flame and soot dynamics are discussed in details, through the study of several soot particles Lagrangian paths.

Finally, an interpretation of the usual time soot intermittency index is proposed in Section 6 based on the full temporal data obtained for the particle size distribution. The results for the corresponding index is then compared with other indexes based on other variables representative of soot particles presence and the obtained differences between them are discussed.

2. Soot sectional model

The soot sectional model is briefly presented here in order to ease its development in the LES formalism. More details can be found in [28,32,33,35] and in Appendix A. The quality of this sectional model on laminar flames is discussed in the Supplementary material of [35].

In the soot sectional approach, the soot particles distribution is discretized in N_{sect} sections. Each section i represents particles with a volume between $v_i^{\min}$ and $v_i^{\max}$, for which the soot mass fraction $Y_{s,i}$ is given by the following transport equation:

$$\frac{\partial \rho Y_{s,i}}{\partial t} + \nabla \cdot (\rho (\mathbf{u} + \mathbf{v_T}) Y_{s,i}) = \rho_s \dot{Q}_{s,i} \tag{1}$$

where ρ is the gas phase density, $\mathbf{u}$ is the gas velocity, $\mathbf{v_T} = -C_{\text{th}} \frac{\nu}{T} \nabla T$ [36] is the thermophoretic velocity (with $C_{\text{th}} = 0.554$), and ρ_s is the constant soot density (chosen equal to $\rho_s = 1860$ kg/m^3). $\dot{Q}_{s,i} = \rho \dot{q}_{s,i}$ is the production rate (in s^{-1}) of the soot volume fraction for the ith section. Diffusion of soot particles is here neglected since soot particles are characterized by high Schmidt numbers [4].

The production rate $\dot{q}_{s,i}$ (in m^3 kg^{-1} s^{-1}) of the soot volume fraction for the ith section accounts for [16,23,35]:

- nucleation (subscript $_{\text{nu}}$), considered as the coalescence of two dimers,
- condensation (subscript $_{\text{cond}}$), considered as the coalescence of a dimer at a soot particle surface,
- surface growth (subscript $_{\text{sg}}$) and oxidation (subscript $_{\text{ox}}$), describing the surface reactivity of soot particles,
- coagulation (subscript $_{\text{coag}}$), corresponding to the collision of two solid particles resulting in a bigger soot particle.

It can then be expressed as:

$$\dot{q}_{s,i} = \dot{q}_{\text{nu},i} + \dot{q}_{\text{cond},i} + \dot{q}_{\text{sg},i} + \dot{q}_{\text{ox},i} + \dot{q}_{\text{coag},i}. \tag{2}$$

The different soot section source terms for nucleation, condensation, surface growth, oxidation, and coagulation are gathered in Appendix A. It is convenient to rewrite all the source terms as a product of two contributions, in order to highlight their dependence on the gaseous and solid characteristics:

$$\begin{aligned}
\dot{q}_{\text{nu},i} &= \dot{q}^{\text{gas}}_{\text{nu},i} \dot{q}^{\text{solid}}_{\text{nu},i} \\
\dot{q}_{\text{cond},i} &= \dot{q}^{\text{gas}}_{\text{cond},i} \dot{q}^{\text{solid}}_{\text{cond},i} \\
\dot{q}_{\text{sg},i} &= \dot{q}^{\text{gas}}_{\text{sg},i} \dot{q}^{\text{solid}}_{\text{sg},i} \\
\dot{q}_{\text{ox},i} &= \dot{q}^{\text{gas}}_{\text{ox},i} \dot{q}^{\text{solid}}_{\text{ox},i} \\
\dot{q}_{\text{coag},i} &= \dot{q}^{\text{fm,gas}}_{\text{coag},i} \dot{q}^{\text{fm,solid}}_{\text{coag},i} + \dot{q}^{\text{c1,gas}}_{\text{coag},i} \dot{q}^{\text{c1,solid}}_{\text{coag},i} + \dot{q}^{\text{c2,gas}}_{\text{coag},i} \dot{q}^{\text{c2,solid}}_{\text{coag},i}
\end{aligned} \tag{3}$$

where the superscripts $^{\text{gas}}$ and $^{\text{solid}}$ correspond to the gaseous and soot dependence parts of each soot source term, which are detailed in Appendix A. It should be noted that the gaseous contribution parts depend only on T, ρ, the dynamic viscosity μ, the pressure P, and the HACA-RC mechanism involved species concentrations [39,40].

2.1. Particle size distribution discretization

Inside each section i, the soot volume fraction density $q(v)$ is considered constant and equal to $q_i = q(v_i^{\text{mean}})$ with $v_i^{\text{mean}} = (v_i^{\min} + v_i^{\max})/2$. The volume particle number density $n(v)$ for each section is then evaluated for $v \in [v_i^{\min}, v_i^{\max}]$ through $n(v) = q_i/v$. The total soot volume fraction f_V and particle number density N_{part} are evaluated as:

$$f_V = \int_0^\infty q(v)dv \quad \text{and} \quad N_{\text{part}} = \int_0^\infty n(v)dv. \tag{4}$$

The particle size distribution discretization is done as follows:

- The first section is defined so that it contains all the nascent particles generated from the collisions of dimers of different sizes, depending on the number of PAHs considered,
- For $i \in [\![2, N_{\text{sect}} - 1]\!]$, the volume intervals of the sections follow a geometrical progression:

$$\begin{aligned}
v_i^{\max} &= v_1^{\max} \left(\frac{v^{\text{MAX}}}{v_1^{\max}} \right)^{\dfrac{i-1}{N_{\text{sect}}-2}} \\
v_i^{\min} &= v_{i-1}^{\max}
\end{aligned} \tag{5}$$

- The last section can be considered as a “trash” section which contains very big unexpected soot particles from v^{MAX} to v^{BIG} and guarantees soot mass conservation. The value of v^{BIG} is chosen as an unattainable soot particle volume. The value of v^{MAX} corresponds to a characteristic volume of the expected biggest soot particles and is chosen as the maximum soot particle volume resolved accurately.