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Soot particles inception and PAH condensation modelling applied in a soot model utilizing a sectional method

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ABSTRACT

This work aims at improving the understanding of soot formation in laminar premixed flames with a strong focus on the interactions between soot and polycyclic aromatic hydrocarbons. In this context, a soot model based on a sectional method is presented. It includes sub-models for the five main processes involved in soot formation and evolution: particle inception, condensation, coagulation, oxidation and surface growth. The two sub-models including novelties are the particle inception and the condensation ones. The nucleation sub-model proposed in the present paper is based on a dampening factor. Concerning condensation, a model taking into account its reversibility is presented and studied.

This model is then validated against experimental data. Five premixed laminar flames have been selected for that purpose. They give insights into the model's ability to predict soot formation depending on fuel, pressure and equivalence ratio. The model predictions show a good agreement with the experimental data concerning soot volume fractions as well as mean particle diameters. The influence of the modelling parameters is also studied. The reversibility of condensation appears to turn condensation into a soot consuming process which may have a significant impact on PAH profiles in premixed laminar flames.

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1. Introduction

Reducing soot emission from comb'ustion-based devices is a major issue for energy and transportation industries because of the growing concerns about soot effects on health, environment and climate [1,2]. More specifically, the smallest particles have been identified as the most harmful to humans [3]. Therefore, a better understanding of soot formation and evolution during combustion events is required.

Various modelling strategies have been proposed for this purpose. Most recent models aim at describing phenomenologically the evolution of the soot number density function (SNDF), usually by solving a population balance equation (PBE). They consider that five main phenomena are driving the formation, growth, and oxidation of soot particles. These phenomena split into two types. The first type comprises the collisional phenomena which are: particle inception from precursors' collisions, condensation which is the name given to soot growth in size due to precursor-soot collisions and soot coagulation. The second type consists of the soot surface reactions, both increasing and decreasing soot particle size. However, the questions raised by Singh et al. [4] about soot particles inception, sticking probabilities of collisional phenomena and active sites on soot surface available for gas-surface reactions are still relevant and studied in recent works [5–11].

The present article focuses on nucleation and condensation (soot growth in size due to precursors collisions on soot particles). More than the processes themselves, the species involved in these processes are yet unknown. According to the literature, these processes are usually connected to large polycyclic aromatic hydrocarbons (PAH) [11–15]. However, the determination of the PAH involved in the actual processes is still an open topic [6–8,16] that is discussed below.

In order to improve the understanding of soot formation, several experimental works have been done by Desgroux and co-workers concerning low-pressure premixed laminar methane flames. Benzene, naphthalene and pyrene have been measured for various equivalence ratios and pressures in sooting flames by Wartel et al. [17,18] using jet-cooled laser induced fluorescence (JCLIF) techniques developed for this purpose in Mercier et al. [19]. These species have been selected because of their importance in the PAH growth pathways. Based on these experimental observations [17,18], El Bakali et al. [20] proposed a detailed gas-phase reaction mechanism describing methane combustion chemistry up to four-ring aromatics. The authors attributed PAH reformation in the burned gases region observed in the sooting flame exclusively to gas-phase endothermic reactions. These new pathways predicted

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benzene and naphthalene profiles in very good agreement with the measurements, whereas the model overestimated pyrene mole fraction in the post-flame region. Mouton et al. [21] also measured soot volume fraction (f_v) measured using laser induced incandescence (LII) in similar flames. The work presented in Mouton et al. [21] also extend the previous studies by performing similar species measurements on a new case, the so-called *nucleation flame* at the very limit of the sooting conditions with an equivalence ratio $\phi = 1.95$. The latest study from Mouton et al. [22] also provided measurements of the fluoranthene profiles. Measurements of the LII decay-times have also been exploited in a joint work presented by Bladh et al. [23] to compute soot primary particles mean diameter profiles. Finally, a study of Desgroux et al. [24] focusing on Mouton et al. [21,22] flame conditions provided novel analysis in order to emphasize the specific sooting behaviour of the lowest equivalence ratio flame called the *nucleation flame*.

First soot modelling results of these flames are included in [21,24]. These results are obtained using the method of moments code provided in [25]. Although the prediction of both the f_v at 40 mm height after burner (HAB) and the soot particles mean diameter are in good agreement with the experimental observations, the predicted f_v profiles shape are significantly different from the measured ones. The computed profiles slopes usually increase with HAB while the observed ones are usually constant or decreasing, sometimes leading to a plateau of the f_v profile, in the burned gases region. Even if uncertainties exist on current f_v measurements in flames, these profiles shapes are commonly observed in ethylene and alkanes flames [21,26–31]. The predicted profiles shapes are driven by nucleation, condensation and chemical surface growth. The presence of pyrene, the species on which nucleation is based on in [24], all along the flame maintains the nucleation rate to be at least similar to the one in the first soot formation region. Therefore, the growing amount of pyrene in the burned gases region would also lead to an increasing nucleation rate responsible for the predicted f_v slope increase in the *nucleation flame*. Even if pyrene is contested as a soot precursor, the measurements previously mentioned concerning benzene, naphthalene, and fluoranthene make it reasonable to think that larger PAH profiles would be similar and grow with HAB in the burned gases region. In the case of sooting flames, chemical surface growth is usually the dominant process. The predicted f_v shape convexity is then explained by the fact that this process is dependent on the soot surface available which is mainly increased by chemical surface growth. In ethylene flame simulations, this aspect is limited by soot surface dehydrogenation, usually in the form of a multiplicative variable deriving from a steady state assumption, limiting the surface reaction. However, this is included in the code used [25] and it does not correct the f_v profile shape in methane flames.

The ability to reproduce the f_v profile shape and the PAH reformation in the burned gases region being not yet satisfactory, new approaches had to be integrated into the combustion chemistry and soot models. The observation of Siegmann et al. [32] that the largest PAH appear after the soot formation in laminar diffusion methane flame inspired the proposed approach. Indeed, such phenomenon would both tend to limit the growth of f_v and increases the PAH formation in the burned gases region. However, instead of creating a general PAH desorption from soot model, the recently considered reversibility of PAH dimerization has been used. The ability of several PAH to form a thermodynamically stable dimer has been studied based on molecular dynamic simulations performed in several recent studies [5,6,33]. Wang [34] proposed to interpret this type results as a potential reversibility of PAH dimerization. This approach was first introduced in a soot model by Eaves et al. [35] for simulations of a Santoro burner flames using a sectional approach. The impact of nucleation and condensation reversibility on f_v and soot number density (SND) were significant. More works, including sensitivity analysis of the model parameters, comparisons with measured particle size distribution function (PSDF) on laminar premixed ethylene flames and numerical comparisons of the influence of various PAH were performed using this approach by the same team [16,36]. However, these promising results are always based on a description of the gaseous phase validated without any effect of the soot model. Moreover, not all precursors used are validated and these gaseous phase validations are performed on cases that are different than the ones the soot model is validated on.

Motivated by the issues mentioned previously, an approach allowing to represent the effect of PAH addition reversibility is proposed in the present paper. Since this study involves condensation reversibility which is a process extruding soot mass from the solid phase such as oxidation, a sectional approach is preferred. Indeed, this type of process can be described by the method of moment, but this topic is still very new and subject to very recent progress [37]. The proposed model is thus based on the sectional approach described in Aubagnac-Karkar et al. [38] with modifications on nucleation and condensation sub-models described in this article.

This paper aims to assess the model's ability to take into account these two processes reversibility while having consistent predictions of both soot indicators (f_v and mean diameter) and the PAH considered as the nucleating species. The laminar methane flames measured by Desgroux and co-workers [21–24] at 200 Torr are used as an experimental reference to that purpose. The *nucleation flame* is chosen for this study because it isolates the influence of the nucleation model. The sooting methane laminar flame chosen is the one at $\phi = 2.32$. This flame provides conditions that are very different from the *nucleation flame* since the measured f_v are four orders of magnitude larger than the ones of the *nucleation flame*. Three more flames have been selected in order to verify the model's ability to reproduce f_v and particle diameter in cases closer to the current literature standards. The atmospheric ethylene premixed laminar flames reported by Xu et al. [31] have been selected. They are flames listed by the International Sooting Flame (ISF) Workshop and their measured f_v are seven orders of magnitude larger than the *nucleation flame* ones.

The constraint on PAH validation restricts the nucleating species choice. Indeed, even if nucleation is argued to be related to fivering or larger aromatics [7,8], experimental data on such species are very scarce in flame conditions. Therefore, pyrene dimerization is used as the nucleating process. Even if this process is unlikely to be the main source of soot particle inception [6–8,39], pyrene concentration evolution has been shown to influence soot formation directly [11,13–15,38,40,41]. Having experimental measurements of both pyrene and f_v in two of the simulated flames allows assessing pyrene-based nucleation validity. However, the proposed process should be considered as a global reaction instead of a description of the actual physical nucleation phenomenon.

A discussion concerning the current possibility to model soot particle inception and mass growth by PAH addition is proposed first in the present paper. It includes a presentation of recent works concerning soot nucleation reversibility and collision efficiency as well as the proposition of new dampening factor for soot nucleation based on the equilibrium constant usually computed for nucleation reversibility. Then, the rest of the soot model and the sectional method used are described. Finally, the validation cases are presented, followed by their simulations' results which are discussed last. The simulations' results part includes parametric variations in order to evaluate the results sensitivity to modelling parameters. A phenomenological analysis of the results based on the source term profiles is also given to complete the results interpretation.

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