Numerical Simulation of Soot Formation in a Turbulent Flame with a Monte-Carlo PDF Approach and Detailed Chemistry

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Abstract

The paper presents an original work in which a hybrid turbulent combustion model, based upon a stochastic evaluation of the Joint Scalar Probability Density Function (PDF), is used in conjunction with a skeletal soot model and a detailed kinetic mechanism for fuel oxidation. After a validation step of the soot model in rich premixed laminar flames, the hybrid Eulerian-Lagrangian approach is applied to predict soot levels in a turbulent jet diffusion flame of ethylene burning in still air. Results are in good agreement with experimental data and the peak value of soot volume fraction on the centerline is fairly well described even though an accurate radiant heat model is still necessary to be more predictive on mean temperature levels.

1 Introduction

With the enforcement of strict environmental regulations, gas turbines and engines manufacturers have been carrying out experimental and numerical works on turbulent reactive flows in order to better understand the very complex phenomena governing the formation of pollutants in flames. Among the unwanted species found in exhaust gases from a turbine combustor, soot has received a great attention [1-2] since it may decrease combustion efficiency ; it also notably influences radiative transfer by enhancing heat exchange with the walls and increasing the visibility of military engines.

With the aim of accurately computing soot particle levels in turbulent reactive flows, a numerical tool has been developed, tested and applied to several flame configurations, including a complex 3D industrial combustor. The paper first presents the approach used to model the challenging issue of chemistry/turbulence interaction. As it is possible with this method to handle detailed kinetic schemes, a comprehensive soot model which incorporates all the known basic phenomena leading to soot particles formation and oxidation is proposed and validated in rich laminar premixed flames at different pressure levels. Then, the solver is applied to compute the main features of the flow, the temperature, the species mass fractions and the soot variables in an ethylene-air turbulent diffusion flame.

2 The turbulent combustion model : a hybrid Eulerian-Lagrangian PDF approach

Predicting the formation of pollutants or, more generally, the levels of minor species in turbulent flames is a complex issue because chemistry time scales usually spread over a large domain and cannot be clearly uncoupled from the physical time scales related to turbulent structures. For more than a decade, it has been shown that Probability Density Functions (PDF) methods [3-4] can be a promising way to deal with the broad range of Damköhler numbers encountered in a typical reactive flow.

Solving the transport equation for the joint velocity-composition PDF [5] may be an interesting way, but we preferred taking advantage from the conventional modelling of turbulence by coupling a classical Reynolds Averaged Navier-Stokes (RANS) solver with a Monte Carlo resolution of the transport equation for the joint scalar PDF. Consequently, the mean flow is computed with the help of the k-ε model while production rates in the species balance equations are evaluated through the Lagrangian procedure involved in the Monte Carlo resolution. This hybrid Eulerian-Lagrangian method (called PEUL+ model) is not completely original since it has been applied to model simple hydrogen and methane flames [6], but using this approach to compute soot levels with a detailed scheme constitutes a new step.

The displacement equation for the fluid particles in the physical space is chosen to respect both Eulerian and Lagrangian velocity spatial correlations whereas the micro-mixing term is closed with the classical IEM model. A particular attention is given to the treatment of the particles seeding in order to get a good statistical convergence in a large number of cells.

3 The soot model and its validation

Concerning soot chemistry, recent works using new experimental techniques have contributed to better understand the complex physics governing the formation and destruction of soot particles in hydrocarbon flames. Simple realistic models have been proposed in order to tackle this issue [7-8], but they often consist of global expressions which apparently restrict their domain of validity. Other models, based upon very detailed chemistry [9-10], give promising results in laminar flames for a wide range of experimental conditions, but they still remain too complicated to be implemented in an industrial code.

Here, an original model of soot formation/destruction, which takes into account all the identified basic mechanisms, is presented and coupled to the Monte-Carlo PDF model in conjunction with a kinetic scheme for fuel oxidation. As we restrict, in a first step, our attention to ethylene-air flames, a 37 species – 124 reactions mechanism [11] is retained to represent the combustion process and the formation of the first aromatic rings (C_6H_6). The pathway to soot is initiated with the formation of the lightest Polycyclic Aromatic Hydrocarbons (PAHs) which are then subjected to a growth process due to acetylene addition and an oxidation process by O_2 and OH attack. In order to reduce computational costs while preserving the complex dynamics of soot formation, only two classes of PAHs are considered in the model. Coalescence between two heavy precursors is the basic step leading to soot inception. Then, particles may coagulate, grow by C_2H_2 addition, collide with a PAH molecule or be oxidised by O_2 or OH radicals. All these mechanisms are accounted for in the present approach.

The soot model was validated against experimental data [12] in rich premixed laminar flames configurations which were already computed in [13] with sophisticated modelling. Two cases (P = 1 bar ; P = 10 bar) were investigated with a 1D laminar flame solver which was modified to incorporate the soot model. Figures 1 and 2 show the predicted profiles for soot variables and soot production rates respectively. Agreements seem to be correct for the soot volume fraction in both cases, showing an accurate behaviour of the model. As expected, surface processes – surface growth and oxidation – play a major role in the particle mass evolution

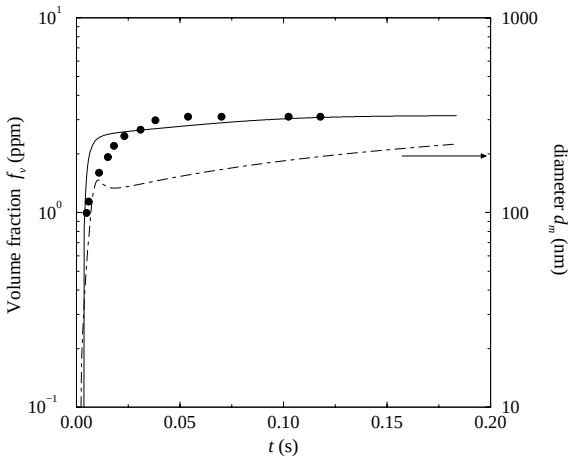

Fig 1. Soot volume fraction and particle diameter profiles for the flame of Bonig et *al* at P = 10 bar

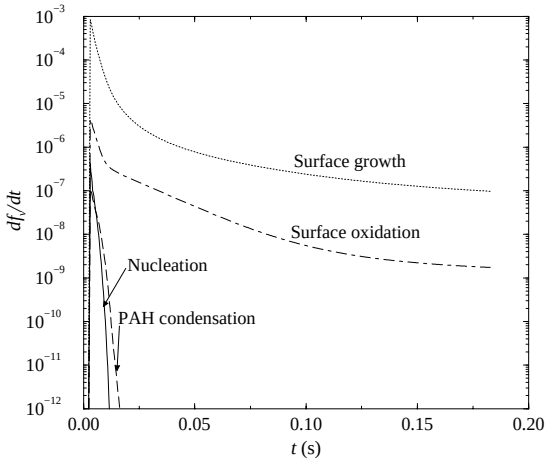

Fig 2. Contributions to soot formation in the flame of Bonig et *al* at P = 10 bar.

4 Simulation of a turbulent jet diffusion flame

In order to assess the hybrid turbulent combustion model coupled to the soot model, a numerical simulation of an ethylene-air turbulent diffusion flame [14] was performed. Flamelet models have already been used in the same type of configuration [15], but here, the full chemistry can be directly incorporated into the flow computation. The evaluation of heat losses due to radiant heat transfer is a crucial issue and cannot be neglected. To date, temperature predictions in turbulent sooty flames with conventional radiant heat modelling are not satisfactory. So, we used a semi-empirical sink term in the Eulerian energy equation to fit the experimental mean

temperature data. Note that the full chemistry Monte-Carlo resolution was only performed as a post-processing procedure in order to avoid expensive computations. The influence of the total number of injected fluid Monte-Carlo particles was investigated and results are shown for mean values and variances of temperature, species mass fractions and soot variables.

Scatter plots of soot volume fractions versus mixture fraction and temperature confirm that soot concentration is poorly correlated to the local equivalence ratio. Figure 3 presents the soot volume fraction profiles on the centerline obtained with 4,000 and 12,000 particles. Absolute levels seem to be in good agreement with experimental values. Moreover, the location of the maximum is fairly well predicted with this approach, which would probably not be the case if fast chemistry assumptions were employed for the intermediate gaseous species, like C_2H_2. The full chemistry model predicts a slower consumption of acetylene on the axis (Fig. 4) which obviously leads to a better estimation of the soot volume fraction peak value. Further analyses (Fig. 5) show that this maximum is determined in the flame brush by a balance between surface growth and oxidation by molecular oxygen and OH radicals.

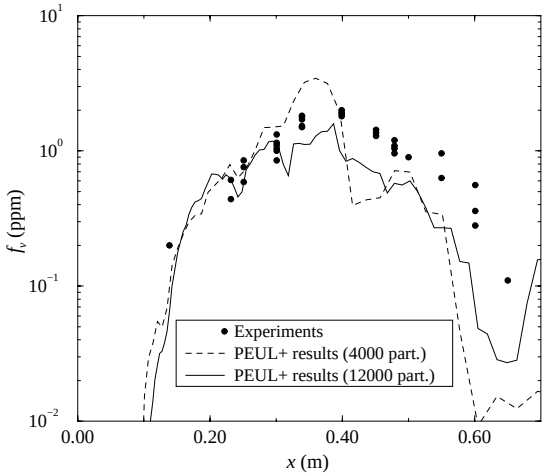

Fig 3 : Soot volume fraction profiles on the jet centerline

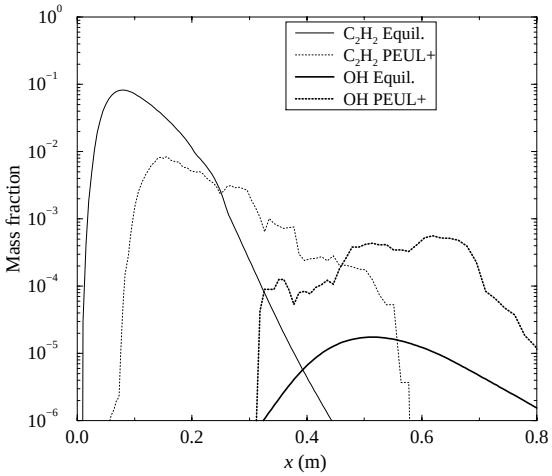

Fig 4 : C_2H_2 and OH mass fractions on the jet centerline computed with PEUL+ compared to the equilibrium assumption

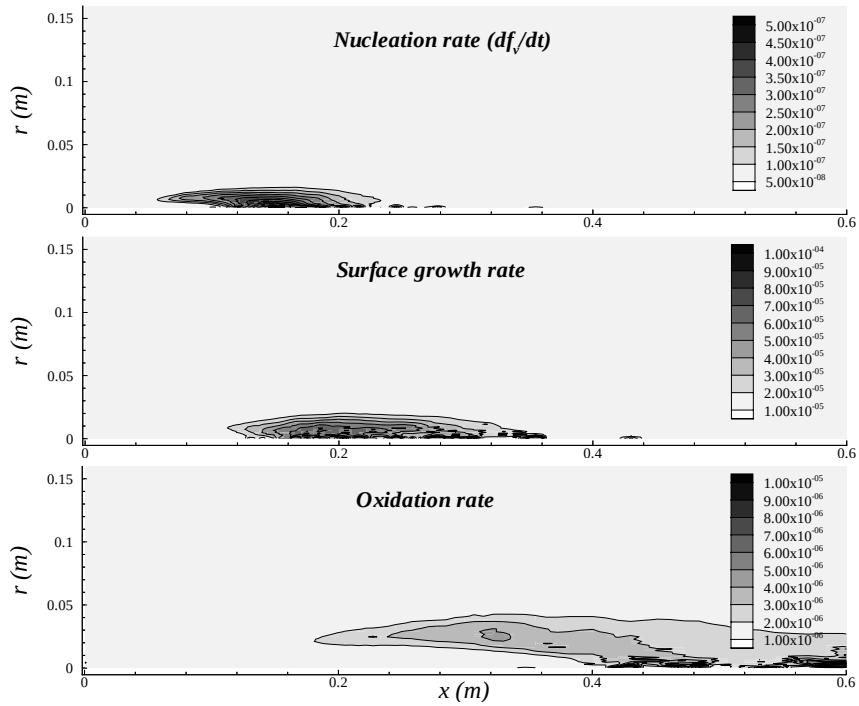

Fig 5. Mean soot production rates inside the flame

5 Conclusions

Hybrid Eulerian Lagrangian PDF turbulent combustion models appear to be good candidates to solve the difficult problem of turbulence/chemistry interaction. Such a model is used here to simulate a turbulent sooty flame with a skeletal approach for soot particles formation and oxidation. Results are encouraging, showing good trends in the different zones of the flame. It also appears that some chemical time scales associated with the fuel decomposition at high equivalence ratios are rather slow compared to the turbulent structure. The flamelet assumption, often used to compute soot levels in turbulent flows, may therefore become questionable. However, the mean temperature prediction is still a crucial problem in this type of configuration, and the coupling with an efficient radiative transfer model has to be done.

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