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# Large eddy simulation of soot formation in a turbulent non-premixed jet flame

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ABSTRACT

A recently developed subgrid model for soot dynamics [H. El-Asrag, T. Lu, C.K. Law, S. Menon, Combust. Flame 150 (2007) 108–126] is used to study the soot formation in a non-premixed turbulent flame. The model allows coupling between reaction, diffusion and soot (including soot diffusion and thermophoretic forces) processes in the subgrid domain without requiring ad hoc filtering or model parameter adjustments. The combined model includes the entire process, from the initial phase, when the soot nucleus diameter is much smaller than the mean free path, to the final phase, after coagulation and aggregation, where it can be considered in the continuum regime. A relatively detailed but reduced kinetics for ethylene–air is used to simulate an experimentally studied non-premixed ethylene/air jet diffusion flame. Acetylene is used as a soot precursor species. The soot volume fraction order of magnitude, the location of its maxima, and the soot particle size distribution are all captured reasonably. Along the centerline, an initial region dominated by nucleation and surface growth is established followed by an oxidation region. The diffusion effect is found to be most important in the nucleation regime, while the thermophoretic forces become more influential downstream of the potential core in the oxidation zone. The particle size distribution shows a log–normal distribution in the nucleation region, and a more Gaussian like distribution further downstream. Limitations of the current approach and possible solution strategies are also discussed.



## 1. Introduction

Most of the current practical combustion systems operate in the non-premixed mode with hydrocarbon fuels. These hydrocarbon fuels (Jet-A, JP-8, etc.) have high carbon and hydrogen content, and hence a high propensity to form soot particles. In gas turbine engines the effect of these solid particles is multi-fold. As the soot particles are generated, they can either oxidize completely or escape oxidation in the form of solid particles. These escaping solid particles can form soot aggregates with diameters in the order of 10 μm for ethylene air flames [1]. If these large solid particles collide with the high speed rotating turbine blades, they can damage the blades' profile and impact upon its lifetime. Moreover, in supersonic military and transport aircraft, usually an afterburner is utilized. Since supersonic aircraft operates in the stratosphere, the soot emitted from the afterburner exhaust will directly impact upon the ozone layer depletion. On the ground, the soot emitted from diesel and gas turbine engines is considered a serious health hazard, since both polycyclic aromatic hydrocarbons (PAHs) that are the main soot precursors, and soot associated organics have been identified as carcinogenic emission.

During combustion, soot formation processes can also affect the production rate of other pollutants, such as carbon monoxide (CO) and nitrogen oxides ($NO_x$) [2], and this is an area that has not been well studied yet. The transport of soot can alter other species concentrations by the surface growth and the oxidation processes. As a result, the local equivalence ratio, the temperature, and the heat release profiles can change. In addition, the high emissivity of soot particles reduces the available chemical energy for conversion into mechanical energy, which results in a loss in combustion efficiency (estimated to be around 30%) [3]. Soot also affects the flame visibility and structure.

Soot formation and modeling within a turbulent environment is one of the least investigated and understood combustion areas. Only few available numerical modeling efforts and experimental data are available in the literature. The poorly understood chemical pathways (which may vary from one fuel to another) and the uncertainty about the coupling between fluid dynamics, heat transfer, kinetics and turbulence, all contribute to the overall uncertainty. In addition, the flow-chemistry interactions encompass a wide range of spatial and temporal scales, which exacerbates the problem and makes it very difficult to perform fully resolved computations for realistic setups. In general, past soot models can be

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classified into two general categories. The most popular approach solves two transport equations for the soot volume fraction and the number density in conjunction with other simplified turbulent models. The second approach uses either a prescribed soot probability density function (PDF) distribution or solves the transport moment equations for the soot PDF.

Most of the early studies of soot formation were in the context of steady state modeling. In one of the earliest numerical study [4] investigated soot behavior in a turbulent acetylene ($C_2H_2$) jet flame using the eddy breakup model for combustion closure. They observed that large soot aggregates are formed inside large turbulent eddies where the residence time is long enough to allow for the slow process of soot formation. Regardless of the over simplification in the closure employed, this study provided a variety of soot oxidation and nucleation models, and showed for the first time how soot chemistry can be integrated in a turbulent environment.

Later studies [5,6] used the laminar flamelet approach combined with the soot mass fraction and the number density transport equation to study a low turbulent buoyant fire and an axisymmetric turbulent methane–air jet flames at elevated and atmospheric pressure. They included radiation by tabulating the local properties in terms of the mixture fraction and the fractional radiative heat loss. Their results showed the importance of radiative heat losses in the prediction of soot, and that the correlation between the soot particles and their oxidizing species (represented by the mean mixture fraction and its fluctuation) influences soot growth rate and its subsequent burnout. For instance, their results show two orders of magnitude under-prediction in soot volume fraction, if the soot properties are uncorrelated with those of the gas phase. This reflects the importance of the coupling between soot and its oxidizing and surface growth species. More recently, Watanabe et al. [7] studied the effect of radiation on spray and soot formation in a two-dimensional DNS study. The same soot model used by Brookes and Moss [6] was combined with the discrete ordinate method to account for radiation. Soot was found to be overestimated in the absence of radiation.

Another mixture fraction based model is the conditional moment closure (CMC) used by Kronenburg et al. [8] to study turbulent methane jet flames. They used a detailed hydrocarbon mechanism and obtained good agreement with measurements. They studied the effect of differential diffusion on soot. They concluded that the assumption of unity Lewis number under-predicts the soot volume fraction by about 40%. The soot differential diffusion effect redistributes the soot particles, such that higher concentration occurs near the centerline in the vicinity of the nozzle and away from the centerline far downstream. This soot redistribution affects its production and destruction rates. The same conclusion was presented by Yunardi et al. [9] for a sooting ethylene–air flames using the CMC approach.

Kollmann et al. [10] applied a detailed soot model along with a joint transported PDF equation of the mixture fraction, enthalpy and soot volume fraction to study an ethylene–air jet flame. They found that most of the soot is formed around 1400 K, and that for such flame the correlation between the mixture fraction and the soot volume fraction is very weak. Recently, Aksit and Moss [11] developed a hybrid model that uses a Lagrangian Monte Carlo solution of the joint scalar PDF of the mixture fraction, soot number density and volume fraction combined with an Eulerian solution of the turbulent flow field. The model used the laminar flamelet-state relationship for the gas phase properties. The model showed good agreement in temperature but an under-prediction of the soot volume fraction along the centerline. The results further showed that the radiation effect is to increase the soot volume fraction. Wen et al. [12] developed a soot model that combines the $k$–$\epsilon$ model for the turbulent flow field with the stretched laminar flamelet approach for a detailed kerosene/air mechanism. They used two soot inception models, one based on acetylene and the another model based on the formation of aromatic rings. They concluded that the acetylene model significantly under-predict the soot volume fraction, which indicate the importance of the aromatic species as an intermediate species in such kerosene/air flame type.

A PDF based transport study was done by Hong et al. [13]. They applied a skeletal $n$-heptane chemistry model with an assumed log–normal soot size distribution in the KIVA-3V code. Their results show good agreement with experimental data of a high pressure shock tube. They concluded that the correct description of the soot formation, as well as the soot transport processes, is critical for achieving reliable predictions. Lindstedt and Louloudi [14] used the method of moment (MOM) combined with a joint-scalar transport PDF to predict the soot properties for two ethylene turbulent flames with full chemistry. Although preferential diffusion effect was not included, their chemistry model includes the surface reactions and PAH formation. They performed two simulations, one with two moments only included and another one that solves up to the third moment. While using two moments over predicts the soot volume fraction, better results were obtained by including the third moment.

Lignell et al. [15] recently used direct numerical simulation (DNS) to investigate the effect of flame structure on soot formation and transport in a two-dimensional turbulent non-premixed flame. The study utilized the same chemical mechanism employed here combined with the transport equations of soot volume fraction and number density. They emphasized the importance of soot differential diffusion and noticed its effect on distributing the soot over a wide range of mixture fraction space. This study [15] along with the current and previous work [16,17] are some of first DNS and LES efforts to simulate soot formation in unsteady turbulent flames.

In the current study, we focus on ethylene–air jet flames and consider acetylene as the primary precursor species for soot formation. There are some experimental data on soot formation in ethylene jet flames. For example, soot volume fraction and temperature have been measured in turbulent ethylene–air flames [18,19]. Results show that the soot production rate is influenced by turbulent mixing, whereas, buoyancy effect reduces soot formation. Other experimental and numerical works have also been reported in the past [20,21].

For the current study, we focus on a more recent set of experiments [22,23]. The experimental measurements provide mean temperature, mean soot volume fraction at the centerline and at a few radial locations. The first work by Hu et al. [22] used thermophoretic sampling followed by transmission electron microscope (TEM) and laser extinction (LE) techniques to provide mean soot volume fraction were used subsequently [23].

The paper is organized as follows. Section 2 provides a brief description of the formulation and models since most of the details are given in a recent paper [16]. Section 3 discusses the numerical set up and test conditions and this is followed by detailed results and discussion in Section 4. Finally, discussion of the limitations of the current model within LES approach and directions for possible improvements will be described.

## 2. Mathematical formulation

The details of the numerical approach and its mathematical formulation can be found elsewhere [16]. Here, a brief review is provided for completeness. In the current work the LES equations in the unsteady and compressible formulation are discretized using a finite volume approach that is second-order accurate in time and space [24]. The space filtered LES equations contain many subgrid terms that require closure. The closure of the subgrid stresses