# Effect of precursors and radiation on soot formation in turbulent diffusion flame

Manedhar Reddy [a], Ashoke De [a,*], Rakesh Yadav [b]

[a] Department of Aerospace Engineering, Indian Institute of Technology, Kanpur 208016, India
[b] Ansys Fluent India Pvt. Ltd., Pune 411057, India

**A B S T R A C T**

Soot formation in 'Delft Flame III', a pilot stabilized turbulent diffusion flame burning natural gas/air, is investigated using ANSYS FLUENT by considering two different approaches for soot inception. In the first approach soot inception is based on the formation rate of acetylene, while the second approach considers the formation rate of two and three-ringed aromatics to describe the soot inception (Hall et al., 1997). Transport equations are solved for soot mass fraction and radical nuclei concentration to describe inception, coagulation, surface growth, and oxidation processes. The turbulent–chemistry interactions and soot precursors are described by the steady laminar flamelet model (SLFM). Two chemical mechanisms GRI 3.0 (Gregory et al.) and POLIMI (Ranzi et al., 2012) are used to represent the effect of species concentration on soot formation. The radiative properties of the medium are included based on the non-gray modeling approach by considering four factious gases; the weighted sum of gray gas (WSGGM) approach is used to model the absorption coefficient. The effect of soot on radiative transfer is modeled in terms of effective absorption coefficient of the medium. A beta probability density function ($\beta$-PDF) in terms of normalized temperature is used to describe the effect of turbulence on soot formation. The results clearly elucidate the strong effect of radiation and species concentration on soot volume fraction predictions. Due to increase in radiative heat loss with soot, flame temperature decreases slightly. The inclusion of ethylene has less synergic effect than that of both benzene and ethylene. Both cases have less impact on the nucleation of soot. The increase in soot volume fraction with soot–turbulence interaction is in consistence with the DNS predictions.

## 1. Introduction

Soot formation and oxidation phenomenology mechanisms have undergone several strides toward making accurate quantitative estimates in combustion systems. There is considerable advance in the predictive capabilities, but complete understanding of the physics and chemistry still persists. To improve the understanding of soot formation detailed modeling is required in order to explain the production of Polycyclic Aromatic Hydrocarbons (PAH), the building blocks of soot. In addition, detailed modeling can be used to provide details regarding the number, size and shape of the particles. Soot formation involves highly non-linear physical and chemical processes. The evolution process of soot has been reviewed by Haynes and Wagner [4], Bockhorn [5], Kennedy [6] and have been classified into four major sub processes. The formation of PAH, conglomeration of PAH, surface reaction of

particles (growth and oxidation) and agglomeration of particles. The accurate modeling of this sub processes is required for the accurate estimation of soot evolution. Modeling soot formation in turbulent diffusion flames is particularly a challenging task due to the small scale interactions between turbulence, chemistry and soot particle dynamics. Description of soot precursors such as acetylene and PAH by the combustion model imposes additional constraints as it involves the resolution of a large number of reactions involving stiff chemistry. Considering radiative heat transfer further increases the complexity, as it affects the kinetic rate associated with soot precursors and creates a two way coupling between combustion and soot models. Soot has high temporal and spatial intermittency due to non-linear interactions between turbulence, molecular transport and chemistry.

The soot nucleation and growth was considered as a first-order function of acetylene concentrations by Brooks and Moss [7], the model was applied to a pilot stabilized turbulent diffusion methane/air flame and reasonable good predictions were obtained. Kronenburg et al. [8] investigated the effect of

* Corresponding author. Tel.: +91 51 2597863; fax: +91 512 2597561.
E-mail address: ashoke@iitk.ac.in (A. De).

turbulence–chemistry interaction on the same flame by using conditional moment closure instead of the extended laminar flamelet model as used in the work of Brooks and Moss. A comprehensive RANS study was performed by Pitsch et al. [9], in this approach a moment method was used to calculate soot evolution. The results were in good agreement with the experimental measurements. The H-Abstraction–Carbon-Addition (HACA) mechanism, is based on the concentration of acetylene only, has sometimes under estimated the soot formation rate, indicating the importance of odd-carbon chemistries like, propargyl ($C_3H_3$), cyclopentadienyl ($C_5H_5$) and benzyl ($C_7H_7$) on the PAH and soot formation rate. Propargyl recombination is considered one of the dominant paths in the formation of benzene. The recent LES study by Mueller et al. [10] on soot formation in Delft Flame III indicated the presence of significant uncertainty in the PAH chemistry. The soot volume fraction was found to be sensitive to the sub-filter variance and showed qualitative agreement with the experimental intermittency. In recent DNS studies, the interaction of turbulence and soot was investigated in terms of transport properties and the evolution of PAH was also studied. The role of transport properties was emphasized by Lignell et al. [11], the work highlighted that the probability of soot moving toward or away from the flame had the same probability. Bisetti et al. [12] used a soot inception model based on PAH instead of an acetylene based model as used by Lignell et al. [11]. It was observed that soot was sensitive to the scalar dissipation rate, this result in intermittency of soot and the slow chemistry results in significant unsteady kinetic effects.

The resolution of chemistry involving soot formation is difficult as it involves the resolution of large number of stiff reactions. Hence mixture fraction based approaches are generally applied. The objective of the present study are (i) to investigate the effect of species concentration and radiation on soot evolution; (ii) to estimate the synergy effect of ethylene and benzene on soot nucleation and surface growth, in addition study the influence of PAH based inception model on soot evolution; and (iii) to study the effect of soot–turbulence interaction on soot evolution process. Different approaches for prediction the OH radical concentration has been examined and their effect on soot formation has been discussed. The results are compared with the experimental measurements of Qamar et al. [13] in order to shed light on the understanding of soot formation in this flame.

## 2. Numerical details

### 2.1. Governing equations

The Favre averaged governing equations of mass, momentum, energy and turbulence are solved which has the following general form as:

$$\frac{\partial}{\partial t}\rho\tilde{\phi} + \frac{\partial}{\partial x_j}\rho\tilde{u}_j\tilde{\phi} = \frac{\partial}{\partial x_j}\rho D\frac{\partial\tilde{\phi}}{\partial x_j} + \langle S_\phi\rangle \tag{1}$$

where the Favre averaged velocity in the $j$th coordinate direction is represented by $\tilde{u}_j$, and $\rho$ is the mean density. The Favre averaged scalar in the turbulent flow filed is given by $\tilde{\phi}$ and $\langle S_\phi\rangle$ represents the mean scalar term of the scalar and $D$ is the coefficient of scalar diffusion. The turbulence scale information is provided by the RSM model.

### 2.2. Turbulence–chemistry interactions

The laminar flamelet model considers the turbulent flame as an ensemble of laminar and one dimensional local structures [14]. The flame surface is defined as an iso-surface of the mixture fraction within the turbulent flow field. Counter flow configuration of laminar diffusion flame is used to represent the thin reactive–diffusive layers in the turbulent flow field. The flame equations can be transformed from physical to mixture fraction space to represent the reactive–diffusive layer and are given by:

$$\frac{\partial Y_i}{\partial t} = \frac{1}{2}\chi\rho\frac{\partial^2 Y_i}{\partial f^2} + S_i \tag{2}$$

$$\rho\frac{\partial T}{\partial t} = \frac{1}{2}\rho\chi\frac{\partial^2 T}{\partial f^2} - \frac{1}{C_p}\sum_i H_i S_i + \frac{1}{2C_p}\rho\chi\left[\frac{\partial C_p}{\partial f} + \sum_i C_{p,i}\frac{\partial Y_i}{\partial f}\right]\frac{\partial T}{\partial f} \tag{3}$$

The mixture fraction and scalar dissipation can be used to map species mass fraction and temperature from mixture fraction space to physical space. The scalar dissipation rate quantifies the deviation from equilibrium and is defined as:

$$\chi = 2D\left|\frac{\partial f}{\partial x_j}\right|^2 \tag{4}$$

The scalar dissipation rate varies along the flamelet and is modeled as Eq. [5] with a small stoichiometric mixture fraction [15] and variable density as:

$$\chi_{st} = \frac{a}{4\pi}\frac{3\left(\sqrt{\rho_\infty/\rho_{st}}+1\right)^2}{\left(2\sqrt{\rho_\infty/\rho_{st}}+1\right)}\left\{-2[erfc^{-1}(2f_{st})]^2\right\} \tag{5}$$

The ensemble of diffusion flamelets are used to represent the turbulent flame brush. The Favre averaged species mass fraction and temperature for a turbulent flame can be determined as:

$$\tilde{\phi} = \iint \phi(f,\chi_{st})p(f,\chi_{st})dfd\chi_{st} \tag{6}$$

where a presumed $\beta$-PDF, used to define the probability of the mixture fraction. The temperature and mean density have an extra