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Effects of aromatic chemistry-turbulence interactions on soot formation in a turbulent non-premixed flame

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Abstract

In this paper, Large Eddy Simulations (LES) have been performed on an ethylene/air piloted turbulent non-premixed sooting jet flame to quantify the importance of aromatic chemistry-turbulence interactions. Aromatic species are of primary importance since their concentrations control directly the soot nucleation rates. In the current work, the chemistry-turbulence interactions for benzene and naphthalene are taken into account by solving transport equations for their mass fractions. A recently developed relaxation model is used to provide closure for their chemical source terms. The effects of turbulent unsteadiness on soot yield and distribution are highlighted by comparing the LES results with a separate LES using tabulated chemistry for all species including the aromatic species. Results from both simulations are compared to experimental measurements. Overall, it is shown that turbulent unsteady effects are of critical importance for the accurate prediction of not only the inception locations, but also the magnitude and fluctuations of soot.

Keywords: Large eddy simulation; Soot; Turbulent non-premixed flames; Chemistry-turbulence interactions

1. Introduction

Due to the detrimental effects of soot emission on human health and the environment, ever more stringent international regulations placed on industrial combustion system emissions make the design of cleaner and more efficient combustion devices a necessity. Towards this end, substantial research efforts are devoted to the numerical prediction of soot formation in turbulent reacting flows [1–3]. Soot nucleates from Polycyclic Aromatic Hydrocarbons (PAH), which involve complex chemical kinetics [4,5]. Incorporating such a detailed chemical mechanism containing hundreds of species and thousands of reactions into three-dimensional turbulent flow simulations using a finite-rate chemistry model is limited by the current capability of computing power.

In this context, tabulated chemistry based on the non-premixed flamelet model [6,7] is an attractive alternative to finite-rate chemistry, and has been a popular modeling approach to simulate numerically turbulent flames [8–12]. The distinct advantage offered by the flamelet model,

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compared to finite-rate chemistry, is that flow properties and chemical kinetics are essentially decoupled [13]. More specifically, flamelet equations are solved in advance to build flamelet libraries, from which species mass fractions, temperature, and other thermochemical properties are evaluated in the flow simulations.

One substantial simplification made by the flamelet model is that the characteristic chemical time scales are much smaller than those of turbulence. In other words, chemistry is assumed to respond infinitely fast to turbulent perturbations. Such assumption has been shown to be valid for the major chemical species (reactants and products) as well as radicals H, OH, O, *etc.*) [14]. However, due to the large time scales characterizing the PAH chemistry, transient effects could be substantial [14,15]. Previous studies have shown that the concentrations of PAH in turbulent non-premixed flames deviate from those predicted by the flamelet model [1]. These observed differences are believed to be a consequence of the rapidly changing turbulent flow field and the slow adjustment of PAH chemistry [1]. Based on the above considerations, unsteady turbulence-chemistry interaction needs to be properly treated for PAH molecules.

Transient effects for PAH molecules have been included first in Large Eddy Simulations (LES) by Mueller and Pitsch [15]. They proposed to solve a transport equation for a lumped PAH variable. The chemical source term of this variable was closed using the same relaxation model as proposed by Ihme and Pitsch [16] for NO_x, which relies on a reversible one-step global reaction. Only the unsteady evolution of the chemical consumption rate of PAH was taken into account [15]. Recently, a conceptually similar, but physically more reliable relaxation model for aromatic species has been proposed and validated based on the chemical response of the unsteady flamelet equations to turbulent perturbations [14]. This new model relies on a multi-step process and distinguishes between major PAH species. The unsteady evolution of both chemical consumption and production terms is included.

Although chemistry-turbulence interactions for aromatic species have already been included in LES, their effects and importance have never been investigated. The objective of this work is to investigate the effects of the aromatic chemistry-turbulence interactions on the formation and later evolution of PAH and soot. Particular attention is paid to the inception locations, magnitude and fluctuations of aromatic species and soot.

This paper is organized as follows. Section 2 describes the models used for combustion, LES closure, PAH, and soot transport. In Sections 3 and 4, the presented models are applied to the LES of an ethylene/air turbulent non-premixed jet flame.

2. Numerical algorithms

The proposed simulation framework relies on four major components: a gas-phase chemistry model, a turbulence closure model, a PAH relaxation model, and finally a soot model.

2.1. Gas-phase chemistry model

In the current work, the combustion processes are described using the flamelet/progress variable (FPV) approach [11], extended to include radiative heat losses in the limit of optically thin medium, similar to [16]. The local thermochemical quantities ϕ are parametrized using three variables, namely mixture fraction Z, progress variable C, and an enthalpy loss parameter H

$$\phi = \mathfrak{F}(Z, C, H), \tag{1}$$

where C is defined as the sum of the mass fractions of CO_2, CO, H_2O, and H_2 [16]. Assuming unity Lewis number [8,10,17], the transport equations for these variables can be written as

$$\frac{\partial \rho \xi}{\partial t} + \nabla \cdot (\rho \xi \mathbf{u}) = \nabla \cdot (\rho D \nabla \xi) + \dot{\omega}_{\xi}, \tag{2}$$

where ξ represents $Z, C,$ and H. The radiation source term for the enthalpy loss parameter includes contributions from both gas-phase and soot radiation. Gas-phase radiation is evaluated using the RADCAL model [18], and soot radiation is modeled following [19]. The database for chemistry tabulation is generated using solutions to the flamelet equations [20]. Source terms, species mass fractions, and other thermochemical quantities are pre-computed and stored. Further details of the FPV approach can be obtained from [15,16].

2.2. LES closure

In this LES, the continuity, momentum, and scalar transport (Eqs. (2)) are filtered spatially. All subfilter stresses and scalar fluxes are closed using a dynamic Smagorinsky model [21–23] with Lagrangian averaging techniques [24,25]. The filtered thermochemical quantities are obtained from the equation of state (Eq. (1)) by convolution with a joint subfilter PDF $\widetilde{P}$

$$\widetilde{\phi} = \iiint \mathfrak{F}(Z, C, H)\widetilde{P}(Z, C, H) dZ dC dH. \tag{3}$$

Since $Z, C,$ and H are not statistically independent variables, a different formulation, equivalent to the above equation, is used in practice

$$\widetilde{\phi} = \iiint \mathfrak{G}(Z, \Lambda, \Theta)\widetilde{P'}(Z, \Lambda, \Theta) dZ d\Lambda d\Theta, \tag{4}$$

with $\Lambda = C(Z_{st})$ and $\Theta = H(Z_{st})$ being mixture-fraction-independent variables. In Eq. (4),