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Damköhler number effects on soot formation and growth in turbulent nonpremixed flames

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Abstract

The effect of Damköhler number on turbulent nonpremixed sooting flames is investigated via large scale direct numerical simulation in three-dimensional *n*-heptane/air jet flames at a jet Reynolds number of 15,000 and at three different Damköhler numbers. A reduced chemical mechanism, which includes the soot precursor naphthalene, and a high-order method of moments are employed. At the highest Damköhler number, local extinction is negligible, while flames holes are observed in the two lowest Damköhler number cases. Compared to temperature and other species controlled by fuel oxidation chemistry, naphthalene is found to be affected more significantly by the Damköhler number. Consequently, the overall soot mass fraction decreases by more than one order of magnitude for a fourfold decrease of the Damköhler number. On the contrary, the overall number density of soot particles is approximately the same, but its distribution in mixture fraction space is different in the three cases. The total soot mass growth rate is found to be proportional to the Damköhler number. In the two lowest Da number cases, soot leakage across the flame is observed. Leveraging Lagrangian statistics, it is concluded that soot leakage is due to patches of soot that cross the stoichiometric surface through flame holes. These results show the leading order effects of turbulent mixing in controlling the dynamics of soot in turbulent flames.

Keywords: Direct numerical simulations; Soot; Damköhler number effects; Turbulent flames; Soot leakage

1. Introduction

Soot emissions are an undesirable byproduct of rich combustion in technical combustion devices such as internal combustion engines, jet engines, and industrial burners [1]. Studies addressing the formation and growth of soot in flames have mostly focused on laminar configurations, for which well-controlled flow conditions enable detailed analysis of soot dynamics [2]. Due to complications in methods and diagnostics brought by the unsteady, three-dimensional turbulent flow field, soot formation in turbulent flames has received significantly less attention [3–11]. Direct numerical simulation (DNS) of turbulent

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combustion coupled with various models for soot formation has been employed successfully to investigate the evolution of soot in turbulent flames [4–7,9,11].

Recently, Bisetti et al. [9] and Attili et al. [11] performed the first two- and three-dimensional direct simulations of turbulent sooting flames employing a high-order statistical model of soot and a chemical mechanism which includes naphthalene, one of the Polycyclic Aromatic Hydrocarbons (PAH) which are recognized as the precursors of soot inception and growth. The authors' results highlight the role of turbulent mixing in controlling the formation of soot precursors and soot, as the local concentration of precursors is very sensitive to scalar dissipation rate. In regions of high dissipation rate, the concentrations of PAH decreases by several orders of magnitude and soot growth is suppressed. In addition, soot drifts in mixture fraction space due to its high Schmidt number compared to that of gas-phase scalars. Therefore, soot parcels meandering across the turbulent flame encounter regions of temperature and composition that promote (or suppress) soot growth.

In the present work, the recent results by Attili et al. [11] are extended in a parametric study varying Damköhler number and keeping Reynolds number constant. Two additional flames are considered with decreasing Damköhler number with respect to the base case value $\mathrm{Da_H}$ in Ref. [11]: $\mathrm{Da_M} = \mathrm{Da_H}/2$ and $\mathrm{Da_L} = \mathrm{Da_H}/4$. The Damköhler number is varied by rescaling all velocities and lengths. This approach is akin to that employed in experiments of jet flames [8] and counterflow burners [12,13] where the Damköhler number is varied by changing the jet exit velocity and the pipe diameter or the distance between the nozzles. The main objective of this work is the characterization of the response of soot formation and growth in turbulent flames to variations in the turbulence hydrodynamic time scales.

2. Methods and models

The gas phase hydrodynamics are modeled with the reactive, unsteady Navier–Stokes equations in the low Mach number limit [14]. The transport of species mass fractions is described using the Hirschfelder and Curtiss approximation to the diffusive fluxes [15] together with a velocity-correction approach [16] to enforce mass conservation. Soret and Dufour effects are neglected. Combustion is modeled using a reduced mechanism for the oxidation of *n*-heptane comprising 47 species and 290 reactions, based on the detailed mechanism developed by Blanquart et al. [17]. The details on the mechanism reduction and various validation cases relevant to *n*-heptane oxidation and benzene formation are available in Bisetti et al. [9].

Soot particles and aggregates are described by their volume (V) and surface area (S) [18], and the Hybrid Method of Moments (HMOM) of Mueller et al. [19] is adopted to describe the evolution of soot. The bivariate soot moment $M_{x,y}$ is defined as $M_{x,y} = \sum_j V_j^x S_j^y N_j$, where x and y are the moment orders for volume and surface, and V_j, S_j, and N_j are the volume, surface area, and number density of soot aggregates belonging to size class j. Moments evolve according to $\partial M_{x,y}/\partial t + \nabla \cdot (\mathbf{u} M_{x,y}) = \dot{M}_{x,y}$, where $\dot{M}_{x,y}$ is a source term describing aerosol internal processes described below. Soot transport is characterized by a high Schmidt number and diffusive mass fluxes are therefore neglected. As shown by Lignell et al. [20] and Bisetti et al. [9], thermophoretic effects [21] are also negligible in sooting turbulent nonpremixed jet flames.

The soot model considers nucleation [22], coagulation [22], growth (condensation and surface reactions) [22,23], and oxidation of soot particles [24,25]. Particle nucleation involves two naphthalene dimers, a molecular cluster composed of two naphthalene molecules. Dimers may also condense on the surface of existing soot particles (condensation). Growth by surface reactions is described by the H-abstraction/C_2H_2-addition (HACA) mechanism [23]. Soot radiation is neglected in the model employed.

The gas velocity and reactive scalar fields are solved with a conventional finite-difference scheme [26], and the system of advection-reaction equations for soot moments is solved with a Lagrangian particle method [27]. The Lagrangian method overcomes some of the issues in Eulerian grid-based schemes for the advection of moments. These issues include the moment realizability problem related to errors in the advective fluxes [28] and the weak stability and poor accuracy due to the stiffness of source terms and high Schmidt number transport [29]. All length and time scales of momentum and gas-phase scalars are fully resolved. The numerical approach adopted here is best described as a DNS for the evolution of the momentum and gas-phase reactive scalars coupled with a robust and efficient Lagrangian scheme for soot transport. Finally, while the models for the chemistry of PAH and for soot formation and growth are very detailed and state-of-the-art, it is worth noting that uncertainties in the description of these processes are well recognized and are the subject of ongoing research efforts.

3. Flame configuration and Damköhler number scaling

The configuration selected for the study is a temporally evolving planar jet. The oxidizer and

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