



Effects of hydrodynamics and mixing on soot formation and growth in laminar coflow diffusion flames at elevated pressures



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ABSTRACT

The formation, growth, and oxidation of soot are studied in a set of laminar coflow diffusion flames at pressures ranging from 1 to 8 atm. The modeling approach combines detailed finite rate chemical kinetics mechanisms that model the formation of Polycyclic Aromatic Hydrocarbon (PAH) species up to pyrene, and a bivariate method of moments that describes soot particles and aggregates by their volume and surface area. The spatial distribution of soot observed experimentally and that predicted numerically are in good qualitative agreement with the peak soot volume fraction located at the flame tip and soot appearing on the flame wings and closer to the nozzle as pressure increases. A detailed analysis of the effect of hydrodynamics and mixing on soot formation is presented. We show that the scalar dissipation rate is lower for the higher pressure flames, promoting the formation of PAH species and soot. Thus, the observed increase in soot volume fraction across flames with increasing pressure is not due solely to mixture density and kinetics effects, rather is affected by hydrodynamics and mixing processes also. Similarly, our results indicate that the decrease in the scalar dissipation rate contribute to changing the location where soot forms in the flame, with soot formation occurring closer to the nozzle and outward on the flame's wings as pressure increases. Radiative heat losses are found to lower the flame temperature, inducing a reduction of the PAH species and associated rates of soot formation. However, heat losses are responsible for a slightly longer flame, which allows for more soot. The overall effect is a modest variation of soot volume fraction if radiation is included.

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1. Introduction

Soot formation as a result of combustion is a matter of great public concern due to the hazards posed by particulates to health and environment. As most practical combustion devices operate at elevated pressures in order to increase thermodynamic efficiency and power density, it is clearly important to investigate the effect of pressure on soot formation, growth, and soot morphology.

In recent years, soot formation at elevated pressures has been studied in various laboratory-scale laminar flame configurations, including counterflow diffusion flames [1], coflow diffusion flames [2–4], and laminar premixed flames [5]. Soot formation in

flames at elevated pressures is one of the focus areas within the International Sooting Flame (ISF) Workshop [6].

Laminar coflow flames are often used to study soot formation [7] and sooting tendencies of fuels [8,9] because they conform to a canonical configuration for which numerous experimental, theoretical, and numerical results are available. Gülder and coworkers have assembled an extensive experimental database of sooting coflow flames of methane (10–60 atm) [10], ethylene (10–35 atm) [11], ethane (2–33 atm) [12], and n-heptane (2–7 atm) [4]. The authors report spatially resolved measurements of the soot volume fraction and temperatures via spectral soot emission.

In most experimental studies at elevated pressure, the burner is operated at constant mass flow rates of fuel and coflow air and, as the pressure increases, velocities reduce as a result of the increase in density. Experiments document the general trends of coflow sooting flames clearly. As pressure increases, soot volume fraction

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increases significantly throughout the flame and soot forms closer to the nozzle. At high enough pressures, the location of peak soot volume fraction moves from the tip to the wings of the flame.

Kailasanathan et al. [13,14] and Steinmetz et al. [15] have investigated flames of ethylene diluted with nitrogen in a coflow of air at pressures between 1 and 16 atm. These experimental datasets are noteworthy and include temperature measurements at various radial and axial locations [13], mole fractions of key gaseous soot precursors along the flame centerline via quartz-probe sampling followed by gas-chromatographic analysis [13,14], and soot volume fraction and morphology via laser-based, optical techniques [15]. For selected flames, multiple quantities are available from the experiments, thereby providing a comprehensive characterization, which facilitates physics-driven inquiry into the mechanisms of soot formation at pressure as well as model development and assessment. The set of flames are known within the International Sooting Flame (ISF) Workshop as “ISF-3 target flame 2” [6].

Previous studies based on detailed numerical simulations of soot formation in coflow flames [2,3,16,17] have concluded that the increase in soot production with increasing pressure is due to enhanced mixture density and species concentrations [16]. Secondary effects are ascribed to modifications to the gas-phase chemistry (i.e. three-body reactions) and changes to the entrainment rates near the flame base. Additional numerical studies investigated the effect of flame preheating [18], gravity [19], and radiation [20,21].

Recently, numerical studies have focused on the characterization of the processes resulting in the growth of soot particles in coflow flames. Eaves et al. [3,22] simulated soot formation in ethane/air coflow flames. According to their models, the growth of soot particles is due mostly to the condensation of Polycyclic Aromatic Hydrocarbon (PAH) species along the centerline, while the H-abstraction C_2H_2 -addition (HACA) [23] mechanism controls soot growth along the flame wing due to the high concentration of radicals next to the flame sheet. The authors also reported that the relative contribution of HACA-based growth decreases with increasing pressure. The study in Ref. [22] presents a detailed analysis of the sensitivity of the growth rates of soot via HACA and condensation to the numerical treatment of the governing equations at the nozzle's exit plane.

Since laminar coflow flames are used as canonical configurations to study soot formation under well-controlled conditions, it is well recognized that comparisons across flames at increasing pressure need to take into account modifications to the flame's structure. The modifications to coflow flames brought by pressure are discussed in Refs. [2,24–26]. Firstly, flames become narrower due to buoyancy, eventually attaining a pencil-like shape [2,3,26]. Secondly, the height of coflow flames does not vary significantly with pressure when the flames are operated at constant mass flow rate [2,24–26].

When the flame becomes narrower due to buoyancy, the flame's cross-sectional area decreases. Although the velocity at the base of the flame is lower for higher pressures on the account of lower flow rates, the reduction in cross-sectional area further downstream results in a higher acceleration of the fluid on the centerline, offsetting the lower velocities at the nozzle's exit plane. Indeed, Liu et al. [2] showed that the centerline velocity and the flame height remain approximately unchanged with increasing pressure. A detailed analysis may be found in Ref. [2].

These observations support the notion that the residence time, proportional to the ratio of the flame height to the centerline velocity, is the same across the set of flames for increasing pressure. Then, the differences in the flames' soot yields are due to variations in the growth rates of soot only, since the residence time and the flow rates of enthalpy and carbon mass remain constant

across flames. In their review, Karataş and Gülder [7] refer to this feature of coflow flames as the basic premise for the *tractability of the laminar coflow flames at elevated pressures*. The increase in the rates of soot growth with increasing pressure has been attributed to the increase in mixture density and additional kinetics effects related to three-body reactions [2,3,16,17].

In our recent studies on turbulent nonpremixed sooting flames [27–30], we have documented the sensitivity of soot precursors to scalar dissipation rate $\chi = 2\alpha|\nabla Z|^2$, where α is the thermal diffusivity and ∇Z the mixture fraction gradient. In Refs. [27–30], it was shown that the mass fractions of PAH species, e.g. naphthalene, drop by several orders of magnitude as the scalar dissipation rate increases moderately, even at values that are far below the extinction limit of the nonpremixed flame [27–30]. As the formation of soot precursors is inhibited by increasing mixing gradients, soot formation is suppressed also.

In the literature on sooting laminar flames, there exist several experimental studies that point to this mechanism. These studies include work on soot formation in opposed flow (i.e. “Tsuji burner”) [31], counterflow [32], and coflow [33] flames. Experimental observations in counterflow flames [32] are as follows. As the strain rate increases, the volume fraction of soot drops below the detection limit by light scattering. If the strain rate increases further, the concentration of Polycyclic Aromatic Hydrocarbon (PAH) species decreases abruptly as detected qualitatively by laser induced fluorescence (LIF). Finally, should the strain rate increase beyond the extinction limit, the flame extinguishes. Du et al. [32] refer to this mechanism as *aerodynamic suppression of soot*.

As discussed above, when pressure increases, coflow flames become narrower due to buoyancy [26]. As a result, the magnitude of the gradient of mixture fraction ∇Z increases. When pressure increases, the flame temperature increases also. The thermal diffusion coefficient α increases with temperature, but decreases with pressure. As a consequence, as pressure increases, changes in the shape of the flame and in the transport coefficients lead to important changes in the scalar dissipation rate χ .

We shall show that, although the velocity along the centerline and the flame height remain unchanged as pressure increases, the scalar dissipation rate field does not. Thus, variations in the scalar dissipation rate lead to important modifications to the concentrations of the soot precursors and, in turn, to the soot yield. As it will be demonstrated in this paper, this *mixing effect* contributes to the variation of the rates of soot growth together with increasing mixture density.

To the best of our knowledge, the effect of changes in scalar dissipation rate on the soot yield in coflow flames at increasing pressures has never been addressed neither experimentally nor numerically. Due to the strong non-linearity in the response of soot precursors to scalar dissipation as well as the complex coupling between gas-phase transport, soot formation, and radiative heat transfer, a detailed numerical study, such as the one reported here, is an ideal approach to explore this effect and isolate individual mechanisms.

In this work, we focus our attention on the ethylene/air coflow flames investigated experimentally by Kailasanathan et al. [13,14] and Steinmetz et al. [15]. These are laminar coflow flames of ethylene diluted in nitrogen in the pressure range 1–8 atm and are known within the International Sooting Flame (ISF) Workshop as “ISF-3 target flame 2” [6]. To the best of our knowledge, this work reports on the first simulations of these flames.

The variations in the velocity, mixture fraction, and scalar dissipation rate fields brought by increasing pressure are characterized and discussed in detail with regard to scaling laws based on suitable reference quantities and non-dimensional numbers, such as the Reynolds and Grashof numbers. The implications of the scaling of scalar dissipation rate across the set of flames with regard to

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