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Effects of water vapor addition to the air stream on soot formation and flame properties in a laminar coflow ethylene/air diffusion flame

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ABSTRACT

The effects of adding water vapor to the air stream on flame properties and soot volume fraction were investigated numerically in a laminar coflow ethylene/air diffusion flame at atmospheric pressure by solving the fully elliptic conservation equations and using a detailed C_2 reaction mechanism including PAH up to pyrene and detailed thermal and transport properties. Thermal radiation was calculated using the discrete-ordinates method and a statistical narrow-band correlated-*k* based wide band model for the absorption coefficients of CO_2 and H_2O. Soot formation was modeled using a PAH based inception model and the HACA mechanism for surface growth and oxidation. Addition of water vapor significantly reduces radiation heat loss from the flame primarily through reduced soot loading and flame temperature. The added water vapor affects soot formation and flame properties through not only dilution and thermal effects, but also through chemical effect. The chemical effect is as significant as the dilution and thermal effects. The primary pathway for the chemical effect of water vapor is the reverse reaction of $OH + H_2 \leftrightarrow H + H_2O$. Our numerical results confirm that the reduced H radical concentration leads to lower PAH concentrations and consequently lower soot inception rates. In contrast, the radiation effect due to the added water vapor was found to have a minor influence on both flame structure and soot formation in the laminar diffusion flame investigated.

1. Introduction

Understanding the effects of water vapor addition to the oxidizer stream of a diffusion flame is of fundamental interest and great practical importance to combustion applications, such as NO_x emission control [1,2] and fire suppression [3–5]. When water mist is added to a fire or flame it causes extinction through the mechanisms of gas-phase cooling, oxygen dilution, and radiation attenuation [3]. Lentati and Chelliah categorized the effects of water mist on flames as (1) physical effects associated with the specific area of water mist, which affects the trajectory and evaporation process of droplets, (2) thermal effects due to the heat capacity and latent heat of evaporation, and (3) chemical effects due to the enhanced overall three-body recombination reactions and shift in water–gas reactions [6].

It has generally been thought that water suppresses combustion processes mainly through the physical mechanisms, i.e., dilution, evaporation, and thermal capacity difference between water vapor and other major species, in both planar premixed flames [7] and counterflow diffusion flames [5,6] by reducing the flame temperatures and diluting the reactants. These studies found that the direct chemical effects of water vapor on the laminar burning velocity or the extinction strain rate are quite small. Thermal radiation transfer was neglected in these studies and hence the role of radiation absorption by the added water vapor or water droplets was not evaluated. On the other hand, the chemical effects of water vapor on flame temperature, burning velocity, and soot and CO formation in premixed flames and diffusion flame have been demonstrated by Müller-Dethlefs and Schlander [8] and Richard et al. [9].

Although most studies on the effectiveness and mechanisms of water mist suppression of flames were performed experimentally, several numerical studies have also been conducted. Lentati and Chelliah [5] carried out numerical studies of the dynamics of water droplets in counterflow methane/air diffusion flames. They found that the optimal droplet sizes for flame suppression are between 20 and 30 μm. Prasad et al. [10] modeled the interactions between water mist and a coflow laminar methane–air diffusion flame established on a Wolfhard–Parker slot burner by solving the full Navier–Stokes (NS) equations. The focus of their study was the effect of droplet size on the extinction water concentration. Ananth and Mowrey [4] conducted a numerical investigation of the interactions between ultra-fine water mist and an axisymmetric

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laminar coflow propane diffusion flame by solving the unsteady NS equations. Chemical reactions were modeled using the GRI-3.0 reaction mechanism. The emphasis of the study of Ananth and Mowrey [4] was the extinction conditions, not the interactions of water vapor with soot formation and radiation absorption. As a consequence, soot formation was neglected and thermal radiation was treated in a simplified manner using the P_1-approximation and the weighted-sum-of-gray-gases model. There is currently a lack of detailed numerical studies on the relative importance of various effects of water vapor addition on flame, soot and radiative properties in coflow diffusion flames.

Previous numerical studies on combustion suppression using water mist focused on the dynamics of water droplets in the combustion flow field. Nevertheless, little efforts have been made to understand the chemical effects of water vapor on soot formation and other flame properties in spite of the fact that addition of water vapor to a heptane pool fire was shown to inhibit chemically the soot formation process in the experimental study of Richard et al. [9]. The chemical effects of water vapor were investigated numerically by Suh and Atreya [11] by substituting nitrogen in the oxidizer stream by water vapor and argon while keeping the oxygen concentration constant in a counterflow methane diffusion flame. They showed that addition of water vapor to the oxidizer stream increases the flame temperature and promotes OH radical concentration, which in turn lowers CO concentration and enhances CO_2 concentration. The pathways for the chemical effect of H_2O, however, were not identified. Therefore, this work seeks to understand how the added water vapor to the air stream of a laminar coflow ethylene diffusion flame affects the flame, soot and radiative properties by numerical calculations using a detailed reaction mechanism.

Comprehensive models for flame/fire interaction with water mist have in general neglected the radiation absorption/attenuation effect by water droplets and water vapor, although the potential importance of such effect has been noticed by Tseng and Viskanta [12], Yang et al. [13], and Consalvi et al. [14]. The objective of this study is to understand the chemical and radiative effects of water vapor added to the oxidizer stream of a laminar coflow ethylene/air diffusion flame by conducting detailed numerical calculations. Ethylene was considered in this study as a representative hydrocarbon because it is an abundant intermediate species in the pyrolysis and combustion of heavier hydrocarbon fuels and its kinetics model has been well developed. Although water mist is used for fire suppression in practical application, instead of water vapor, the present study concerns water vapor addition to the air stream of a coflow diffusion flame to avoid the complexity of dealing with water droplets. Combustion chemistry was modeled using a detailed mechanism for C_2 hydrocarbon fuels. To account for the radiation absorption effect of the added water vapor and radiation heat transfer in the flame the radiative properties of radiating species, namely CO, CO_2, H_2O and soot were modeled using a statistical narrow-band correlated-k based wide-band model. The chemical effect of the added water vapor on soot formation was investigated using a soot formation model based on collision of polycyclic aromatic hydrocarbons (PAHs) for soot particle inception and the hydrogen abstraction C_2H_2 addition (HACA) mechanism for surface growth and oxidation. The limitation of the present study is that the numerical results are not validated due to the absence of experimental data.

2. Numerical model and solution method

The diffusion flames to be modeled in this study are axisymmetric, atmospheric–pressure, laminar coflow ethylene ones established in the Gülder burner [15] without and with water vapor addition to the oxidizer (air) stream. The burner consists of a fuel tube of inner diameter of 10.9 mm (0.94 mm thickness) surrounded by an 88 mm inner diameter co-annular tube for delivery of coflowing oxidizer.

2.1. Governing equations

The governing equations to be solved are the steady-state fully-coupled elliptic conservation equations for mass, momentum, energy, and species mass fractions in the low Mach number limit and in axisymmetric cylindrical coordinates. These equations have been described in detail in previous studies, e.g., Guo et al. [16], and therefore will not be repeated here. It is worth pointing out that the gravity term is included in the momentum equations and the source term due to thermal radiation transfer is accounted for in the energy equation.

2.2. Radiation model

The radiation model employed in this study has also been well documented in the literature, e.g., Liu et al. [17]. The radiative properties of radiating gases, namely CO, CO_2, and H_2O, were modeled using an optimized 9-band model based on the lumping strategy and the statistical narrow-band correlated-k method [18]. The absorption coefficient of soot was calculated using the Rayleigh expression as $k_s = 5.5 f_v \eta_c$ with f_v being the soot volume fraction and η_c the wavenumber at the band centre. The total radiation intensity over each spectral band is evaluated using the 4-point Gauss–Legendre quadrature scheme. The absorption coefficients at each quadrature point and each band were precalculated and fit as a polynomial function of temperature [18]. The radiative transfer equation in 2D axisymmetric cylindrical coordinates was solved by the discrete-ordinates method (DOM) described in detail in [17]. The T_3 quadrature scheme in cylindrical coordinates, provided in [17], was used for angular coordinate discretization and the spatial discretization was achieved using the central differencing scheme. Further details on the radiation model can be found in [17,18].

2.3. Soot model

Since the acetylene based semi-empirical two-equation soot model proposed by Leung et al. [19] is in general unable to predict the chemical effects of chemically active additives on soot formation, it is necessary to employ a more sophisticated soot formation model to investigate the chemical effect of the added water vapor on the flame properties and soot formation. The soot model employed in this study has been described in detail in Zhang et al. [20] and is only briefly summarized below.

Soot inception is assumed to be the result of collision of two pyrene molecules (A_4). The subsequent surface growth and oxidation are assumed to follow the HACA mechanism [21,22]. The aggregation process of soot particles is modeled using a sectional aerosol dynamics model [20]. In the sectional model each aggregate is assumed to comprise equally sized spherical primary particles and to have the same fractal dimension of 1.8. The mass range of aggregates is divided into a number of discrete sections with prescribed masses. Soot aggregates are assigned into these prescribed sections according to their mass. The nucleation step connects the gaseous incipient species (A_4) with the solid phase. The sectional transport equations for soot aggregates and primary particles can be found in [20]. In this study, 35 sections were used in the sectional model with a spacing factor of 2.35 [20].

Soot nucleation rate is calculated by the collision rate of two pyrene molecules in the free-molecular regime, but enhanced by a factor of 2.2 due to van der Waals force [22]. PAH condensation on soot particles also contributes to the surface growth of soot.