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Review

On the influence of the correlation between enthalpy defect and mixture fraction in sooting turbulent jet flames

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ABSTRACT

The effects of the cross correlation between mixture fraction and enthalpy defect on flames structure and radiative heat transfer are investigated using a hybrid Stochastic Eulerian Field/flamelet model. An ethylene turbulent jet diffusion flame is simulated by considering or not this correlation. Model results show that mixture fraction and enthalpy defect are strongly correlated in the region located downstream the peak of temperature. Neglecting this correlation affects the flame structure in a non-negligible manner in this part of the flame. In addition, the radiative loss and the radiative flux are significantly enhanced when the correlation is disregarded.

Contents

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1. Introduction

An accurate modeling of turbulent flames requires, on the one hand, to consider detailed chemical mechanisms that consider the main reaction pathways and, on the other hand, to model the turbulence-chemistry interactions. The size of the chemical mechanisms increases in a non-linear manner with the number of carbon atom that composes the fuel or with application considered. As an example, in the case of sooting flames, the chemical mechanism has to be sufficiently exhaustive to give access to the intermediate species involved in the production of soot. As a consequence, the large number of chemical species and reactions involved in soot formation and oxidation is prohibitive for solving the species and energy equations simultaneously to the equations which describe the flow field when performing numerical simulation of soot formation with CFD codes.

Under the assumption of widely separated time scales for chemical reactions and transport processes, the combustion chemistry attains a quasi-steady state and adjusts with short relaxation times to local flow conditions. By this, the chemical kinetics can be decoupled from the mixing process. This idea is realized in the flamelet concept [1]. Temperature, species mass fractions and the scalars related to these quantities can be represented by the mixture fraction, ζ, the scalar dissipation rate, χ, which accounts for the influence of the flow field on the flamelet structure, and an enthalpy defect parameter, X_R, that quantifies the radiative loss [2,3]. To determine the moments of these scalars a Probability Density Function (PDF) of (ζ, χ, X_R) [1,4] is then required. In practice, these parameters are assumed to be statistically independent and the PDFs are modeled as a presumed PDF for ζ (a β PDF is often considered) and as a Dirac function for X_R and χ [5–10]. A notable exception in the field of presumed-PDF method is the work of Hartick et al. [11], who generated a two-dimensional PDF of mixture fraction and enthalpy defect from the first and the second moments of these two quantities. Nmira et al. [12] used a transported PDF method to investigate the evolution of the correlation between mixture fraction and enthalpy defect in an oxygen-enhanced jet turbulent flame. They found that mixture fraction and enthalpy defect are correlated over a large part of the flame, suggesting that the assumption of statistical independence is not valid. The objective of this article is to investigate the influence of this correlation on flame structure and radiative heat transfer in an ethylene turbulent jet flame where heat transfer by radiation dominates transfer by conduction and convection in the heavily sooting regions of the flame [13]. To the authors' best knowledge, such an analysis has not been reported in the literature.

This paper is organized as follow: the first part presents the numerical model. The experimental data and results are presented and discussed next. Finally, the concluding remarks are drawn.

2. Numerical model

The physical models and numerical algorithms used here are the same as those used in [14]. The model was validated by simulating 12 sooting turbulent jet flames with a wide range of Reynolds number and fuel sooting propensity [14]. Here only the essential aspects of the models are reviewed. Additional details of the models can be found in [14].

2.1. Turbulent combustion

The Favre-Averaged Navier-Stokes equations in a low Mach number formulation are solved in axisymmetric cylindrical coordinates. The turbulence closure is modeled by means of the standard k-ε model. The enthalpy defect flamelet model (EDFM) is used to obtain state relationships for density, species and temperature as unique functions of ζ, χ, and X_R. The flamelet library is generated using a full chemical kinetic scheme, involving 70 species and 463 reactions, developed by Qin et al. [15]. Enthalpy defect parametrization was introduced using the methodology described by Carbonell et al. [1].

2.2. Soot production

The semi-empirical acetylene/benzene-based two-equation model, proposed by Lindstedt and based on soot mass fraction, Y_S, and soot number density, N_S, is considered [16]. It accounts for the contributions of soot nucleation, surface growth, oxidation by O_2, OH and O and coagulation. The constant adopted for nucleation and surface growth terms are the same as those proposed by Lindstedt except for the pre-exponential factor for the surface growth term, which was set equal to 0.4×10^3 m/s. This adjustment was found to match the experimental peaks of soot volume fraction in a laminar coflow ethylene diffusion flame burning in air [17]. The suitability of this value was confirmed in Ref. [14] where 12 turbulent jet diffusion flames fueled with hydrocarbons covering a wide range of a fuel sooting propensity were simulated. The rate of oxidation by O_2 is given by the NSC model [18], while soot oxidation by OH and O were based on the Fenimore and Jones model [19]. In the present study soot formation and oxidation rates were stored in a flamelet library in the same manner as Carbonell et al. [3].

2.3. Radiative transfer

The radiative participating species considered here are CO_2, H_2O and soot. Soot particles were assumed to be spherical and small as compared with the wavelength, Rayleigh's theory then being applied to obtain the soot absorption coefficient [20]. A wide-band (WB) correlated-k model is used as radiative property model. The spectral coverage range considered in this work is 200–15000 cm^{-1}. The spectrum was divided into $N_{WB}=20$ WBs as follows: 10 WB of 500 cm^{-1} between 200 and 5200 cm^{-1}, 4 WB of 1000 cm^{-1} between 5200 and 9200 cm^{-1}, 1 WB of 800 cm^{-1} between 9200 and 10000 cm^{-1} and 5 WB of 1000 cm^{-1} between 10000 and 15000 cm^{-1}. On each