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Full Length Article

A calibrated soot production model for ethylene inverse diffusion flames at different Oxygen Indexes

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ABSTRACT

A numerical investigation was carried out in order to gain insights into the soot production mechanisms by studying the effect of the oxygen concentration of the oxidant stream, known as Oxygen Index (OI), on soot production and flame radiation in laminar Inverse Diffusion Flames (IDF). Several laminar axisymmetric IDF were simulated, varying the OI from 17% to 35%. All flames were fueled with pure ethylene. Comparisons to experimental data were intended to assess and improve the capabilities of a two-equation acetylene/benzene-based semi-empirical soot production model and a Full-Spectrum correlated-k (FSCK) radiative property model. Higher OI were found to generate shorter flames, presenting higher temperatures and an increase in the soot production and energy irradiated. Results show that simulations predict correctly the experimental behavior observed by changing the OI, but reliable predictions are limited to values under 25%. In order to improve the generality of the results, the soot production model was modified, incorporating the soot surface aging effect in an approximated way on the surface growth mechanism, and then it was calibrated. A square root dependence was considered in the specific soot surface area rather than a linear dependence. A sensitivity analysis shows that the surface growth process is the most sensitive in terms of predicting the soot content produced. Simulations after calibration were in satisfactory agreement with the experimental measurements, presenting accurate predictions from both local and overall points of view. Results demonstrate that IDF is a relevant configuration to obtain insights concerning soot modeling, providing a decoupled oxidation process, similar residence times at different OI, and thermal age controlled by temperature alone. Results also demonstrate that considering an aging effect on the soot surface reactivity is necessary in order to properly model the variations induced by changing the OI.

1. Introduction

Fully understanding the radiation of heat emitted by the flame is one of the key elements that need to be addressed in order to optimize the combustion process in industrial applications. This of course involves consider several aspects of the combustion process that are extremely complex and, at this moment, not completely understood. A configuration that facilitates understanding these phenomena are laminar diffusion flames. This reliable and replicable configuration allows to obtain insights concerning the combustion process, the production of soot particles and other pollutants, and the generation of heat. Besides, laminar diffusion flames are ideal for carrying out both experiments and numerical simulations, avoiding the uncertainties introduced by turbulence. Numerous studies have been carried out in this kind of flames in order to assess the reliability of soot models [1–7] and to study the effects of different parameters on soot production and radiation [8–13]. Despite this large number, only a few have considered studying the Inverse Diffusion Flames (IDF), experimentally [14–21] or numerically [22–24,20]. An IDF is a co-flow flame in which the oxidizer is injected at the central port, while the fuel is injected at the annular section surrounding it. A second outer annular section provides an inert injection, which avoids the fuel to react with the ambient air. This produces a flame with a limited quantity of oxygen available to react with the fuel.

The soot content produced by IDF is very different from the one produced in NDF. Even though the processes associated with its formation seem to be similar, they are subjected to very different conditions. In NDF soot forms in the inner side of the reaction zone, at the fuel-rich side. Then these particles are convected upward to the tip of the flame, where they are oxidized as they pass through the high-temperature oxidation-intensive zone. In IDF the soot also forms in the fuel-rich side, but in this case is located in the outer side of the reaction

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Nomenclature

A_S	soot surface area per unit volume [m^{-1}]
C_a	agglomeration constant
D_ξ	diffusion coefficient [$m^2\ s^{-1}$]
d_p	diameter of the particles [m]
f_S	soot volume fraction
HRR	heat release rate [W]
h	enthalpy [$J\ kg^{-1}$]
h_{ad}	adiabatic enthalpy [$J\ kg^{-1}$]
h_f	flame height [m]
h_u	unburned enthalpy [$J\ kg^{-1}$]
k_i	kinetic constant for reaction rate i
κ_B	Boltzmann constant [$J\ kg^{-1}$]
N_A	Avogadro constant [$part\ mol^{-1}$]
N_S	soot number density [$part\ kg^{-1}$]
N_C	carbon atoms in incipient soot particle
$\dot{q}_R$	radiative flux [$W\ m^{-2}$]
R_f	flame radius [m]
S_{N_S}	source term for soot number density [$part\ m^{-3}\ s^{-1}$]
S_{Y_S}	source term for soot mass fraction [$kg\ m^{-3}\ s^{-1}$]
T	temperature [K]
W_S	soot molecular weight [$kg\ kmol^{-1}$]
X_{rad}	enthalpy defect parameter
x_i	mole fraction of species i
Y_S	soot mass fraction
β	radially integrated soot volume fraction [$ppm\ cm^2$]
ξ	mixture fraction
ρ	density [$kg\ m^{-3}$]
φ_i	collision efficiency factor of i-th process
χ	scalar dissipation rate [s^{-1}]
χ_R	radiant fraction
$\dot{\omega}_i$	reaction rate if i-th process

subscripts

a	agglomeration
ad	adiabatic
coag	coagulation
n	nucleation
S	soot
sg	surface growth
st	stoichiometric

zone. Then these particles are convected out of the high-temperature zone, releasing a high quantity of un-oxidized (unburned) soot particles [23]. Since the soot oxidation process is almost completely reduced in IDF, this particular configuration allows decoupling the soot formation-oxidation competition seen in NDF. This allows better comparing and calibrating the soot production models, focusing in the formation and growth of the soot particles. Better understanding and predicting these processes will allow fine-tuning the combustion at an industrial scale.

One parameter that can be used to optimize the combustion process is the oxygen concentration of the oxidizer flow. This quantity, known as Oxygen Index (OI), affects the stoichiometry of the reaction and then its local temperature. This increase in temperature produces an intensification in the soot formation processes, producing more soot than in normal ambient conditions (21%), but also intensifying the oxidation reactions and therefore the soot consumption [25]. This competition will lead to an intensification in flame radiation at the range of OI studied [26,27], which can be of practical interest in the design of oxy-fuel burners applied to a variety of industrial processes to improve efficiency and pollution characteristics.

Studies carried out comparing the effects of the OI in IDF are very limited. Sidebotham and Glassman [28] studied these effects over the temperature and species concentration for an ethylene IDF. They determined that oxidation processes can play an indirect but significant role on the observed intermediate hydrocarbon species profiles, and therefore on soot formation. Sunderland et al.[14] studied the flame length of ethane NDF and IDF in normal and reduced gravity, leading to increased luminosity, soot production and soot emission for both normal and inverse flames at oxygen-enhanced conditions. Krishnan et al. [19] studied the effect over the radiation properties for also ethane NDF and IDF, showing that oxygen enhancement led to reduced flame lengths, increased luminosity and increased total radiative heat loss for both normal and inverse diffusion flames. Bhatia et al. [24] simulated the flames studied by Sunderland et al. [14], obtaining that the effect of gravity-variation and oxygen enhancement on flame shape and size was far more pronounced for NDF than for IDF. Stelzner et al. [20] carried out an experimental and numerical analysis on an IDF with pure oxygen and diluted CH_4/CO_2. They indicate that near the burner the Soret effect must be considered, while further downstream the self-absorption for the radiating species is important, specially at low scalar dissipation rates.

The present study analyses ten axisymmetric ethylene laminar IDF, varying the OI from 17% to 35%. These flames were compared to experimental results obtained by Escudero et al. [21]. Comparison with these results are intended to assess the capabilities of a numerical model, based on a Steady Laminar Flamelet (SLF) model, a two-equation semi-empirical soot formation model and a Full-Spectrum correlated-k (FSCK) radiative property model. This model was validated over a wide range of laminar axisymmetric diffusion flames, with different fuels and sooting propensities in [10], with a fixed OI of 21%. The present study focuses specifically on the semi-empirical soot production model developed by Lindstedt and used in Refs. [10,29–33]. It provides a simplified description of the soot formation and oxidation processes as compared to the state-of-the-art PAH-based soot models [2,3,6,7]. However, this semi-empirical model captures most aspects of the physical and chemical dynamics of soot formation and evolution in a small set of partial differential equations [10,34], which makes it more easily tractable in industrial applications or fire safety problems involving turbulent flames [29–33]. As an example, this model was applied to simulate a series of turbulent jet diffusion flames fueled by different C1–C3 hydrocarbons covering a wide range of fuel sooting propensities, Reynolds numbers, and ambient conditions in terms of pressure and oxygen concentration in the oxidizer stream, and was found to provide soot volume fraction within a factor of two by using a single set of parameters [32,33]. In a first step the same parameters and the same set of constants as used in [10] are considered to simulate the IDF at different OI. In a second step, a calibration process of the soot production model is performed in order to improve their predictions. This later process takes advantage of the natural decoupling of the soot production mechanisms in IDF easing the analysis.

The aim of the paper is, on the one hand, to assess the capabilities of the soot production model highlighting the advantages of studying different Oxygen Indices (OI) considering an Inverse configuration. From this assessment an improvement to the model was proposed in order to correctly predict the soot content at different OI. For the other hand, the improvement proposed implies that it is necessary to consider the loss in the reactivity of the soot surface growth process, normally called as aging of the soot particles, in order to provide accurate predictions of the soot content.

2. Numerical models

The overall continuity equation, the Navier-Stokes equations in a