Fuel 178 (2016) 37–48

Contents lists available at ScienceDirect

Fuel

journal homepage: www.elsevier.com/locate/fuel

Transported scalar PDF modeling of oxygen-enriched turbulent jet diffusion flames: Soot production and radiative heat transfer

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HIGHLIGHTS

- Transport PDF modeling of oxygen enriched sooting turbulent je flames.
- Oxygen index effects on soot production and radiative heat transfer.
- Fuel sooting propensity effects on radiative heat transfer.
- Non-monotonic evolution of the soot production with increased oxygen index.

ARTICLE INFO

Article history:
Received 16 November 2015
Received in revised form 28 January 2016
Accepted 10 March 2016
Available online 19 March 2016

Keywords:
Turbulent jet diffusion flame
Oxygen index
Propane
Methane/ethylene blend
Soot production
Radiation

ABSTRACT

Turbulent jet flames fueled either by propane or a methane/ethylene blend and burning under different oxygen indexes (OI) in the range from 21% (air) to 100% (pure oxygen), studied experimentally by Wang et al. (2002), were simulated by using an hybrid flamelet/Stochastic Eulerian Field (SEF) method, an acetylene/benzene-based two-equation soot model, and a wide-band correlated-k (WBCK) method to model the spectral dependence of the absorption coefficient of the gaseous radiatively participating species and soot. Emission Turbulent Radiation Interactions (TRIs) are taken into account by means of the PDF method, whereas absorption TRIs are modeled using the optically-thin fluctuation approximation (OTFA). Model predictions in terms of soot volume fraction, radiant heat flux distribution along the wall of the combustion chamber, and radiant fraction are compared with the experimental data of Wang et al. (2002), showing a reasonable agreement. The non-monotonic evolution of the soot production with the OI, increasing sharply when the OI is enhanced from 21% to about 40% and then being significantly reduced as the OI is further increased, and the effects of the fuel sooting propensity, with the propane flames producing much more soot than the methane/ethylene blend flames, are well reproduced by the numerical model. The non-monotonic influence of the OI on soot production can be explained by several competing mechanisms. The soot production tends to be enhanced owing to, on the one hand, the increase in temperature and, on the other hand, a positive feedback between surface growth process and soot surface area observed for moderate level of oxygen enrichment. Oppositely, the soot production tends to be reduced due to a decrease in residence time and an enhancement in the oxidation of both soot precursors and soot particles.

1. Introduction

The use of oxygen-enriched air as an oxidizer offers a number of advantages in combustion applications such as glass furnaces, boilers and incinerators. It improves both the thermal efficiency of the process and the flame stability and leads to a massive reduction in the flue gas volume and in the amount of NOx formed [1]. An important characteristic of oxygen-enhanced combustion is the enhancement of thermal radiation, due to effects on temperature and soot, which improves the performance of the combustion process [1].

The presence of intermediate soot appears then to be desirable to increase radiative heat transfer. This has motivated a significant amount of experimental and numerical works on the influence of the oxygen index, defined as the volume fraction of oxygen in the oxidizer flow and denoted hereafter as OI, on soot production. Most of these studies considered well-defined laminar diffusion

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http://dx.doi.org/10.1016/j.fuel.2016.03.035
0016-2361/

Nomenclature

A_S	soot surface area (m^{-1})
d_n	inner burner diameter (m)
$\tilde{f}_\phi$	Favre PDF of ϕ
f_S	soot volume fraction (–)
$f_{S,EQ}$	equivalent soot volume fraction (–)
g	cumulative k-distribution function
g_k	kth quadrature points
G_η	incident radiation per unit wavenumber ($W\ m^{-1}$)
h	enthalpy ($J\ kg^{-1}$)
I	radiative intensity
I_b	blackbody intensity (Planck function)
k	absorption coefficient variable (m^{-1}) or turbulent kinetic energy ($m^2\ s^{-2}$)
k_S	soot absorptive index (–)
m_S	complex index of refraction for soot (–)
N_F	number of fields
N_G	number of quadrature points
N_S	soot number density per unit mass of mixture ($part\ kg^{-1}$)
n_S	soot refractive index (–)
N_{WB}	number of wide bands
N_α	number of composition variables
$\dot{q}''_{Rw}$	wall radiative flux ($W\ m^{-2}$)
Q'''_R	radiative source term in enthalpy equation ($W\ m^{-3}$)
$\dot{Q}_R$	total radiative loss (W)
r	radial coordinate (m)
T	temperature (K)
u	velocity ($m\ s^{-1}$)
w_k	kth quadrature weight
W_i	molecular weight of the ith species ($kg\ mol^{-1}$)
$\vec{W}$	vector of independent isotropic Wiener processes ($s^{1/2}$)
X_R	enthalpy defect parameter (–)
Y_S	soot mass fraction (–)
z	axial coordinate (m)
χ	scalar dissipation rate (s^{-1})
χ_R	radiant fraction (–)
ε	dissipation rate of the turbulent kinetic energy ($m^2\ s^{-3}$)
η	wavenumber (cm^{-1})
$\vec{\eta}$	vector of random variable (–)
κ	absorption coefficient
μ_t	apparent turbulent viscosity ($kg\ m^{-1}\ s^{-1}$)
ρ	density ($kg\ m^{-3}$)
σ_t	apparent turbulent Prandtl or Schmidt number (–)
$\dot{\omega}$	soot reaction rate ($kg\ m^{-3}\ s^{-1}$)
ψ	sample-space variable corresponding to ϕ
ζ	mixture fraction (–)
Ω	solid angle (–)

Subscript

α	αth scalar
ad	adiabatic
abs	absorption
emi	emission
f	flame
gk	kth quadrature point
i, j	directions i or j
mix	mixing
n	nth field
R	radiation or radiative
S	soot
Sf	soot formation
Sox	soot oxidation
Eq	equivalent
t	turbulent
η	at a given wavenumber or per unit wavenumber

Superscript

i	ith wide band

Operators

$<\phi>$	Reynolds averaged quantity
ϕ'	Reynolds fluctuating quantity
$\tilde{\phi}$	Favre averaged quantity
ϕ''	Favre fluctuating quantity
$\langle A \vert B \rangle$	expectation of the conditional probability of event A given that event B occurs

flames involving either counterflow [2–7] or axisymmetric configurations [8–12]. Experimental studies of counterflow diffusion flames showed that soot production was increased with rising the OI [2–5], thermal effects being identified as the main cause of this enhancement [3,5]. In addition, numerical studies reported the capability of detailed soot formation model [3] and two-equation semi-empirical soot models [4,6,7] to capture this enhancement in soot production. The study of axisymmetric laminar coflow diffusion flames evidenced that increasing the OI affects the soot production through several competitive mechanisms [8]: on the one hand, the enhancement in soot nucleation and growth mechanisms due to the increase in flame temperature is expected to increase the soot concentrations. On the other hand, the increased presence of oxygen promotes oxidative mechanisms and reduces the flame residence times, which tend to decrease the soot concentrations. Lee et al. [8], Zepoulaga et al. [9], and Merchan-Merchan et al. [10] considered methane flames, methane flames doped with acetylene and polycyclic aromatic hydrocarbons (PAH) and biodiesel flames, respectively, and reported that the peak of soot volume fraction evolves in a non-monotonic manner with the OI, increasing with the initial oxygen enhancement up to a maximum and then decreasing as the OI is further increased. These results suggest that the mechanisms that promote soot production dominate for low increase in OI whereas those that tend to suppress soot prevail as the OI is further increased.

Flames encountered in industrial processes are usually turbulent which add difficulties both on experimental and modeling point of view. Wang et al. [13] carried out measurements of soot volume fraction, NOx emission and radiative loss in turbulent jet flames burning under oxygen-enriched environments with OI in the range between 21% and 100%. Three fuels, namely natural gas, propane and a blend of 90% methane/10% ethylene by volume, were considered. The peak of soot volume fraction was found to exhibit the same non-monotonic evolution as function of the OI as reported in axisymmetric laminar diffusion flames [8,10]. Oppositely, the radiative losses were found to increase continuously with the oxygen-enhancement. The fuel-type effects revealed that, for a given OI, the propane flames produce much more soot than the methane/ethylene flames, which produce slightly more soot than the natural-gas flames. In addition, increasing the fuel injection velocity was found to enhance soot production. The simulations of some of these flames have been reported. Wang et al. [14,15] used a RANS approach coupled to an eddy-breakup model to compute the propane flame with an OI of 40% and a Reynolds number of about 15000. They used a detailed reaction mechanism, an advanced PAH-based soot production model and a spectral