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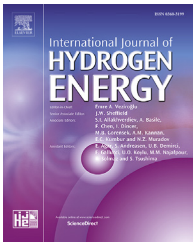

Assessing the role of turbulence-radiation interactions in hydrogen-enriched oxy-methane flames

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ABSTRACT

Statistical analysis of scalar data obtained from single-shot laser measurements in four turbulent oxy-fuel flames were carried out to develop a functional relationship for the temperature self-correlation (TSC) term for use in Turbulence Radiation Interaction (TRI) models. The developed relationship was found to be invariant with the hydrogen enrichment in the fuel, fuel jet Reynolds numbers and correlated reasonably well with the root-mean-square of temperature (T_{rms}). The TSC and the absorption-coefficient temperature correlation (ATC) were both modeled in terms of T_{rms} and employed as add-on functions in time-averaged flame simulations. Including the effects of TRI enhanced the radiant fraction by 40% and reduced outlet CO concentrations by 30% across all flames. Further, there was significant flame absorption due to the high concentrations of radiatively participating gases that would deem optically thin radiation approximations in these flames to be erroneous.

Introduction

Oxygen enhanced combustion can enhance heat transfer rates in industrial heating and melting processes. In addition to increased energy efficiency and productivity, their association with lower pollutant emissions, increases their significance in light of growing environmental regulations. The enhanced heating rates primarily stem from higher temperatures and secondly from the higher total concentrations of the radiatively participating gases (CO_2 and H_2O) due to the absence of Nitrogen [1]. Further, improvements in combustion efficiencies may be obtained by enriching the hydrocarbon fuel stream with hydrogen. This results in higher temperatures and lower CO concentrations due to improved combustion efficiencies. However, an increase in NOx emissions are an undesirable consequence of the resulting high temperatures [2–4]. Computational Fluid Dynamic (CFD) simulations that utilize high-fidelity combustion models to predict the surface heating rates and pollutant formation rates accurately can provide valuable insights towards optimizing industrial furnace operations [1,5,6]. However, it has been well-recognized that time-averaged simulations that ignore the interactions between the turbulence and radiation field can result in a significant underestimation of the radiative fluxes [7–9]. This is because time-averaging the radiative transfer equation (RTE) results in four closure terms [10]. The net result as a result of the interactions between all of the closure terms is an enhancement in the flame emission. Turbulence Radiation Interaction (TRI) model formulations attempt to model these closure terms in terms of the turbulent

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Nomenclature

a	Fraction of blackbody emissive power
G	incident radiation, W/m^2
I	radiative intensity, W/m^2-Sr
k	absorption coefficient, m^{-1}
K_t	Turbulent Kinetic Energy, m^2/s^2
$\mathbf{q}$	radiative heat flux vector, W/m^2
T	temperature, K
w	angular weights

Greek symbols

ε	emissivity
ζ	direction cosine in the x-direction
μ	direction cosine in the y-direction
μ_t	turbulent viscosity, m^2/s
η	direction cosine in the z-direction
σ	Stefan-Boltzmann constant, W/m^2-K^4
ρ	density, kg/m^3
χ_R	total radiative heat loss fraction

Subscripts

b	blackbody
i	gray gas component
m	discrete angular direction of intensity
rms	root-mean-square

scalar fluctuations. The computational cost and complexity in modeling the closure terms have led several authors to quantify and assess the relative importance of each term. This has resulted in TRI models of varying levels of fidelities [8,9,11]. For instance, Prof. Modest and co-workers [12,13] developed TRI models utilizing a compositional Probability density function (PDF) framework to rigorously model the fluctuations of the various TRI terms. However, some experimental evidence have pointed to the fact that the higher order moments of temperature fluctuations may not be that important [14]. Consequently, less rigorous methods where the TRI terms were modeled in terms of the second moment of temperature (Trms) only has also been undertaken [11,15,16]. While one of the ways to establish a functional relationship between the TRI terms and Trms is through a Taylor's series expansion of the emissive power terms [10,11,15], this can also be undertaken using high-fidelity laser measurements of the scalar fluctuations. This has been done by Krishnamoorthy for methane flames (Sandia Flame D) [17] as well as hydrogen flames (Sandia Flame A) [18]. A very strong correlation between the time-averaged emissive power and the intensity of temperature fluctuations was observed in both flames.

Other studies have also determined the temperature self-correlation (TSC) to be the most important TRI term in methane-air flames [8], whereas the absorption coefficient temperature correlation (ATC) was deemed to be equally important at higher flame opacities [9,11]. The importance of absorption coefficient self-correlation on the other hand was close to unity even at higher opacities [9] and was attributed to the fact that while the specie and temperature fluctuations are positively correlated, the absorption coefficient and temperature are negatively correlated. On average, a 30% enhancement in flame emission was observed across all studies due to the inclusion of TRI models. However, in hydrogen enriched oxy-flames, the increased concentrations of the participating gases may further enhance the impact of TRI models by increasing the magnitude of the closure terms involving absorption coefficients and the ATC term in particular. A goal of this manuscript is carry out this assessment.

Single-shot Raman spectroscopic measurements of very high fidelities at a wide range of hydrogen enrichment and fuel jet Reynolds numbers have recently been available to study the extinction characteristics in methane-hydrogen oxy-flames [19]. Although these measurements were intended as a valuable dataset for the validation of turbulence, chemistry and mixing models they can also be used to assess the impacts of TRI closure terms. The overall goal of this manuscript is to utilize this dataset to come up with closure formulations to assess the impact of TRI models in time-averaged CFD simulations. Specifically, answers to the following questions are pursued here:

1. Does the level of hydrogen enrichment have an impact on the functional form of the correlation between the time-averaged emissive power and turbulence fluctuation intensities?
2. Does the fuel jet Reynolds numbers have an impact on the on the functional form of the correlation between the time-averaged emissive power and turbulence fluctuation intensities?
3. In lieu of the high concentrations of the participating gases, what are the relative magnitudes of the temperature-self

Table 1 – Summary of flames studied.

Flame	%mol O_2 in oxidizer	%mol H_2 in fuel	Reynold's number, ref	Jet speed (m/s)	Co-flow speed (m/s)
A1	32	55	15000	98.2	0.778
A2	32	45	15000	84.4	0.755
A3	32	37	15000	75.8	0.739
B3	32	55	18000	117.8	0.933

Table 2 – Summary of physical models employed in the CFD simulations.

Physical models	Primary modeling option
Gas-Phase chemistry	Eddy Dissipation Concept with a 41-step skeletal mechanism (Smooke [24])
Gas-Phase radiative property	WSGGM (5 gg) [23] [a]
Turbulence	Realizable k-ε [22]
Radiative transport equation solver	Discrete ordinates method (Angular resolution, theta x phi: 3 × 3) [22]
Turbulence Radiation Interactions (TRI)[a]	TSC approximation (Eqs. (13) and (14)) TSC + ATC approximation (Eqs. (15) and (16))

[a] These models were implemented as User-Defined Functions (UDFs) in ANSYS FLUENT.

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