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Radiation energy devaluation in diffusion combusting flows of natural gas

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ABSTRACT

Abstract: CFD (Computational fluid dynamics) is used to evaluate the thermodynamic second-law effects of thermal radiation in turbulent diffusion natural gas flames. Radiative heat transfer processes in gas and at solid walls are identified as important causes of energy devaluation in the combusting flows. The thermodynamic role of thermal radiation cannot be neglected when compared to that of heat conduction and convection, mass diffusion, chemical reactions, and viscous dissipation. An energy devaluation number is also defined, with which the optimum fuel–air equivalence for combusting flows can be determined. The optimum fuel–air equivalence ratio for a natural gas flame is determined to be 0.7. The CFD model is validated against experimental measurements.

1. Introduction

Thermal radiation in combustion systems has been studied for different reasons. The energy transfer aspects have received much attention recently. Thermal radiation has also been studied for its role in pollutant emissions. A radiation beam, however, not only transport energy, but also entropy and exergy. The entropy transfer function of a radiation beam was shown by Ref. [16] to be important in solar engineering. While the radiation energy is a conserved quantity, the radiation entropy and radiation exergy are not conserved [16]. These aspects of thermal radiation, while receiving much less attention, may also have significance for large-scale industrial combustion systems.

In combustion systems, entropy generation and exergy losses are traditionally associated with four irreversible processes: viscous dissipation, heat conduction and convection, mass diffusion, and chemical reactions [14]. The entropy generation due to these processes occurring under different combustion modes has been studied in detail recently by Ref. [6]. Theoretically, entropy generation due to thermal radiation also need to be considered for combustion systems, since it is known from past studies (see for instance [22] that these equipments usually involve high-temperature processes in which thermal radiation is the dominant mode of heat transfer.

The importance of entropy generation in combustion systems is that it destroys exergy [21]. Exergy represents that part of the energy, which can be converted into maximum useful work [20]. Since the exergy losses increase with entropy generation, the usual approach for optimizing combustion systems is then to find the conditions which minimize entropy generation [20]. The concept of EGM (entropy generation minimization) is developed and discussed extensively by Refs. [2–4]. However, according to [9]; the importance of entropy generation rests with its effect on the quality of the energy that is being transferred. Since the quality of the transferred energy is reduced through entropy generation [9], proposed using an energy devaluation measure for the performance of thermal systems and processes.

The discussion given by Ref. [9] highlights the functional role of entropy generation in thermal systems and is used as the basis in this study to assess the importance of radiative energy devaluation in a laboratory-scale combusting flow. The radiation entropy generation is computed based on the model recently derived by Ref. [5]. The computations, addressing a 300 kW natural gas-air co-axial diffusion flame were carried out with the FLUENT® 6.3 CFD (computational fluid dynamics) code. The problem definition is shown in Fig. 1. Boundary conditions (except for the fuel inlet flow rate) were derived from experimental data [19].

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Nomenclatures

c_0	speed of light in vacuum, 2.9979 × 10^8 m s^{-1}
$\dot{E}'''_{\mathrm{dev}}$	energy devaluation density, W m^{-3} s^{-1}
h	Planck's constant, 6.6261 × 10^{-34} J s
H	enthalpy, J kg^{-1}
I_λ	spectral radiative intensity, W m^{-3} sr^{-1}
$J_{i,\mathrm{eff}}$	effective mass diffusion flux, kg m^{-2} s^{-1}
k_{b}	Boltzmann's constant, 1.3807 × 10^{-23} J K^{-1}
k_{eff}	effective thermal conductivity, W m^{-2} K^{-1}
L_λ	spectral radiative entropy intensity, W m^{-2} μm^{-1} sr^{-1} K^{-1}
m_{fuel}	mass flow rate of fuel, kg s^{-1}
M_{fuel}	molecular weight of fuel, kg $kmol^{-1}$
$\overline{M}_{\mathrm{W}}$	mean molecular weight, kg $kmol^{-1}$
$\mathbf{n}_w$	unit outward normal vector of a boundary wall
N_{dev}	energy devaluation number
$\dot{Q}$	heat transfer rate during combustion, W
$\mathbf{r}$	unit position vector
$\mathbf{s}$	unit direction vector
$\dot{S}'''_{\mathrm{gen}}$	total local volumetric entropy generation rate, W m^{-3} K^{-1}
$\dot{S}'''_{\mathrm{gen,cc}}$	local volumetric entropy generation rate due to heat conduction and convection, W m^{-3} K^{-1}
$\dot{S}'''_{\mathrm{gen,ch}}$	local volumetric entropy generation rate due to chemical reactions, W m^{-3} K^{-1}
$\dot{S}'''_{\mathrm{gen,f}}$	local volumetric entropy generation rate due to viscous dissipation, W m^{-3} K^{-1}
$\dot{S}'''_{\mathrm{gen,m}}$	local volumetric entropy generation rate due to mass transfer, W m^{-3} K^{-1}
$\dot{S}'''_{\mathrm{gen,r}}$	local volumetric entropy generation rate due to gas radiation processes, W m^{-3} K^{-1}
$\dot{S}''W_{\mathrm{gen,r}}$	local volumetric entropy generation rate due to wall radiation processes, W m^{-3} K^{-1}
$\dot{S}_{\mathrm{G}}$	total entropy generation rate, W K^{-1}
T	temperature, K
T_λ	spectral radiation temperature, K
χ	chemical potential, J kg^{-1}
ε_{W}	emissivity of wall
$\kappa_{\mathrm{a}\lambda}$	spectral absorption coefficient, m^{-1}
$\kappa_{\mathrm{s}\lambda}$	spectral scattering coefficient, m^{-1}
λ	wavelength, m
μ_{eff}	effective viscosity, kg m^{-1} s^{-1}
$\dot{\omega}$	rate of reaction, kmol m^{-3} s^{-1}
Φ	scattering phase function
Ω	solid angle, sr
Ψ	viscous dissipation function for swirling flows, s^{-2}

2. Mathematical formulas and simulation method

2.1. Combusting flow modeling

The combustion process was modeled using the two-step global reaction mechanism given by Ref. [23]:

$$\begin{aligned}&CH_4+(3/2)O_2\rightarrow CO+2H_2O\\&CO+(1/2)O_2\rightarrow CO_2\end{aligned}\tag{1}$$

Temperature dependent properties were considered for all species [24]. The turbulence–chemistry interaction was based on the finite-rate/eddy dissipation model. In his model, both the Arrhenius and eddy-dissipation reaction rates are calculated. The net reaction rate is taken as the minimum of these two rates. In practice, the Arrhenius rate acts as a kinetic “switch”, preventing reaction before the flame holder. Once the flame is ignited, the eddy-dissipation rate is generally smaller than the Arrhenius rate, and reactions are then controlled by turbulent mixing.

The RNG $k-\varepsilon$ turbulence model is accurate for swirling combusting flows [25] and was selected. Radiation was modeled assuming a semitransparent absorbing, emitting and scattering combusting medium with a variable absorption coefficient. The following radiative energy transfer equations were solved using the discrete ordinates method [13]:

$$\frac{\mathrm{d}I_\lambda(\mathbf{r},\mathbf{s})}{\mathrm{d}s}+(\kappa_{\mathrm{a}\lambda}+\kappa_{\mathrm{s}\lambda})I_\lambda(\mathbf{r},\mathbf{s})=\kappa_{\mathrm{a}\lambda}I_{\mathrm{b},\lambda}+\frac{\kappa_{\mathrm{s}\lambda}}{4\pi}\int\limits_{4\pi}I_\lambda(\mathbf{r},\mathbf{s}')\Phi(\mathbf{s}',\mathbf{s})\mathrm{d}\Omega'\tag{2}$$

$$I_\lambda(\mathbf{r}_{\mathrm{W}},\mathbf{s})=\varepsilon_{\mathrm{W}}I_{\mathrm{b},\lambda}(\mathbf{r}_{\mathrm{W}})+\frac{1-\varepsilon_{\mathrm{W}}}{\pi}\int\limits_{\mathbf{n}\cdot\mathbf{s}'<0}I_\lambda(\mathbf{r}_{\mathrm{W}},\mathbf{s}')|\mathbf{n}_{\mathrm{W}}\cdot\mathbf{s}'|\mathrm{d}\Omega'\tag{3}$$

where, λ is wavelength, $\kappa_{\mathrm{a}\lambda}$ is spectral absorption coefficient, $\kappa_{\mathrm{s}\lambda}$ is spectral scattering coefficient, I_λ is spectral radiative intensity, $I_{\mathrm{b}\lambda}$ is blackbody spectral intensity, Φ is the scattering phase function, Ω is solid angle, **s** is a unit position vector, **r** is a unit direction vector, ε_{W} is wall emissivity, and $\mathbf{n}_{\mathrm{W}}$ is a unit normal vector at walls.

A WSGGM (weighted-sum-of-gray-gases model) was used for the absorption coefficient, while the scattering coefficient was assumed to be $\kappa_{\mathrm{s}\lambda}=0.01\ \mathrm{m}^{-1}$. The emissivity at walls was taken from measured data [19].

2.2. Entropy generation in combusting flows

Entropy generation in combusting flows is traditionally associated with four irreversible processes: viscous dissipation, heat conduction and convection, mass diffusion, and chemical reactions [14]. In this study, the thermal radiation effects are added. The total local volumetric entropy generation rate is then computed as follows

$$\dot{S}'''_{\mathrm{gen}}=\dot{S}'''_{\mathrm{gen,ch}}+\dot{S}'''_{\mathrm{gen,m}}+\dot{S}'''_{\mathrm{gen,f}}+\dot{S}'''_{\mathrm{gen,cc}}+\dot{S}'''_{\mathrm{gen,r}}\tag{4}$$

where, $\dot{S}'''_{\mathrm{gen,ch}}$, $\dot{S}'''_{\mathrm{gen,m}}$, $\dot{S}'''_{\mathrm{gen,f}}$, $\dot{S}'''_{\mathrm{gen,cc}}$, and $\dot{S}'''_{\mathrm{gen,r}}$ are the local entropy generation rates due to chemical reactions, mass diffusion, viscous dissipation, heat conduction and convection, and volumetric radiation processes, respectively. They are defined as following:

$$\dot{S}'''_{\mathrm{gen,ch}}=\frac{\sum_i\dot{\omega}(-\Delta H)\overline{M}_{\mathrm{W}}}{T}\tag{5}$$

$$\dot{S}'''_{\mathrm{gen,m}}=-\frac{\sum_i J_{i,\mathrm{eff}}\nabla\chi_i}{T}\tag{6}$$

$$\dot{S}'''_{\mathrm{gen,f}}=\frac{\mu_{\mathrm{eff}}\Psi}{T}\tag{7}$$

$$\dot{S}'''_{\mathrm{gen,cc}}=\frac{k_{\mathrm{eff}}}{T^2}(\nabla T)^2\tag{8}$$