Numerical Simulation of Entropy Generation in Non-Premixed Combustion

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Abstract : This study presents the numerical simulation of the thermodynamic irreversibilities, generated by combustion process in a cylindrical burner. The calculation of the turbulent diffusion flame properties is based on the standard k-ε turbulent model. The simulation considers the contribution of each mechanism in the generation of entropy, i.e. friction, heat conduction, species diffusion and chemical reaction. The computations are performed by the Fluent-CFD package. As results, the chemical reaction and the heat conduction are the major sources of entropy production. Moreover, preheating air reduces significantly thermodynamic irreversibilities within the combustor while air factor has slight negative impact.

Keywords : Entropy generation; Turbulent combustion; Thermodynamic irreversibility; Computational Fluid Dynamics.

1. Introduction

It is recognized by many studies that the combustor is least efficient system in power plants [1-3]. In order to improve the efficiency of the combustion system it is necessary to identity the physical and chemical mechanisms responsible of thermodynamic irreversibilities. The contribution of each mechanism can be determined by calculating its entropy generation [4-6]. Wherefore, the basic equations expressing the distributions of velocity, temperature and species concentrations are used to deduce the local entropy generation rate [7-9]. The review paper of Some and Datta (2008) outlined all the works dealing with computing entropy production in combustion process covering different fuel types (liquid, gaseous and solid), different configurations (confined, unconfined), different flame types (premixed, non-premixed) and different flow regimes (laminar, turbulent). Laminar flames were considered at first by [2, 9-11] showing that the thermal diffusion, chemical reaction, mass diffusion and the viscous dissipation represent in order of enumeration the predominant sources of entropy generation. Few works were interested in turbulent flames despite their fundamental role in actual combustors. Stanciu *et al.* and Yapici *et al.* [1,7, 10-12] works are based on the standard k-ε model for modeling turbulence and strong irreversible chemical reaction assumptions, i.e. one-step or two-steps exothermic reactions or fast-chemistry reaction. The numerical analysis of Yapici *et al.* [6, 7,11] was limited to computing uniquely the thermal and viscous contributions in the entropy generation; the former dominates largely the last. The computation of Stanciu *et al.* divided the entropy field in mean part and turbulent part. The important result is that at whole the turbulent fluctuations are the major source of entropy generation, in decreasing volumetric rate, the mains contributors are chemical, thermal conduction and mass diffusion [1, 10, 12].

The present study is interested in the calculation of thermodynamic irreversibilities occurred in turbulent combustion process in a coaxial jets burner. This combustor configuration was the focus of numerous experimental as well as numerical investigations because its relatively simple geometry and its representativeness of gas turbine burners. The study is based on the k-ε turbulent model and it considers two steps combustion reaction. The local entropy generation rate is calculated taking into account all the mechanisms responsible of entropy generation, i.e. viscous friction, heat conduction, species diffusion and chemical reaction. Besides, the effects of the preheat inlet air and air factor of mixture on entropy generation are analyzed. All the simulations are carried by the software Fluent.

2. Burner Configuration

The present study is a continuation of a previous numerical analysis [13, 14] proposed to support the experimental work [15] interested in turbulent diffusion flames characterization. The burner depicted in Figure 1 and considered in the experimental study consists of a coaxial jets discharging into a cylindrical chamber pressurized to 3.8 atm. The burner is of ray R4=0.06115 and length L=1m and is with isothermal walls of 500K. The fuel (CH_4) is issued from the inner jet with ray R1=0.03157m, with the velocity of 0.987 m/s at temperature of 300K, while the preheated air at temperature T2=750K is supplied from the annular jet of external ray R3= 0.04685m at a velocity of 20.63 m/s.

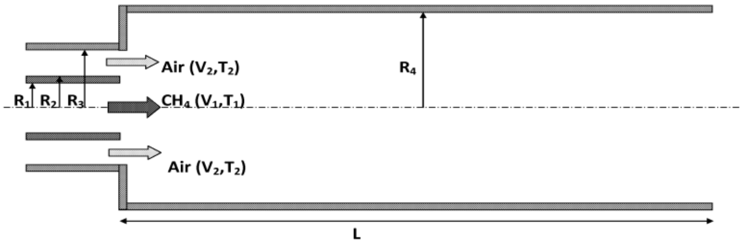

Figure 1. *Schematic of the burner.*

3. Governing Equations

The simulation of combustion in the burner is supposed steady, turbulent and axisymmetric. According to these assumptions, in the following, the set of equations suitable to the adopted combustion model [1,2,10-12]:

Continuity:

$$\frac{\partial}{\partial x_i}(\rho u_i) = 0 \qquad (1)$$

Momentum:

$$\frac{\partial}{\partial x_i}(\rho u_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial xj} \qquad (2)$$

Energy

$$\frac{\partial}{\partial x_i}(\rho u_i h) = u_i \frac{\partial p}{\partial x_i} + \tau_{ij}\frac{\partial u_i}{\partial x_j} + \frac{\partial}{\partial x_i}\lambda_{eff}\frac{\partial T}{\partial x_i} - \frac{\partial}{\partial x_i}\left(\sum_{k=1}^{n}\rho y_k U_{k,i} h_k\right) \qquad (3)$$

Species:

$$\frac{\partial}{\partial x_i}(\bar{\rho}\bar{u}_i y_k) = \frac{\partial^2 \rho D_k y_i}{\partial x^2{}_i} + \dot{\omega}_k \qquad (4)$$

Thermodynamic status:

$$p = \rho RT \sum_{k=1}^{n} \frac{y_i}{M_i} \qquad (5)$$

Turbulence kinetic energy:

$$\frac{\partial}{\partial x_i}(\rho u_i k) = \frac{\partial}{\partial x_j}\left(\mu + \frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j} + G_k - \rho\varepsilon + S_k \ , \qquad (6)$$

Dissipation rate:

$$\frac{\partial}{\partial x_i}(\rho u_i \varepsilon) = \frac{\partial}{\partial x_j}\left(\mu + \frac{\mu_t}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_i} + C_{1\varepsilon}\frac{\varepsilon}{k}G_\varepsilon - C_{2\varepsilon}\rho\frac{\varepsilon}{k} + S_\varepsilon \, . \qquad (7)$$

Where: $C_{1\varepsilon} = 1.44, C_{2\varepsilon} = 1.92, \sigma_k = 1.0, \sigma_\varepsilon = 1.3$.

The combustion reaction is modeled with a two-steps reaction mechanism where the production and the combustion of carbon monoxide (*CO*) are taken into account. In the first stage, methane is oxidized into carbon monoxide and water vapor, but in the second, carbon monoxide is oxidized into carbon dioxide. The reaction mechanism takes place according to the constraints of chemistry, and is defined by stoichiometric equations [2&11]:

Reaction 1:

$$CH_4 + \frac{3}{2}O_2 \rightarrow CO + 2H_2O \qquad \text{(step 1),} \qquad (8.a)$$

Reaction 2:

$$CO + \frac{1}{2}O_2 \rightarrow CO_2 \qquad \text{(step2).} \qquad (8.b)$$

Once the computations achieved, the results obtained will be exploited to calculate the local entropy generation rate [2, 7,10-12]:

$$\dot{S}_{gen} = (\dot{S}_{gen})_f + (\dot{S}_{gen})_h + (\dot{S}_{gen})_d + (\dot{S}_{gen})_{ch} \ , \qquad (9)$$

Where:

$(\dot{S}_{gen})_f$: Fluid friction volumetric entropy generation, $$(\dot{S}_{gen})_f = \frac{\mu_{eff}}{T}\frac{\partial u_i}{\partial x_j}\frac{\partial u_i}{\partial x_j} > 0 \tag{10}$$

$(\dot{S}_{gen})_h$: Heat transfer volumetric entropy generation, $$(\dot{S}_{gen})_h = \frac{\lambda_{eff}}{T^2}\frac{\partial T}{\partial x_j}\frac{\partial T}{\partial x_j} > 0 \tag{11}$$

$(\dot{S}_{gen})_d$: Diffusion of species volumetric entropy generation, $$(\dot{S}_{gen})_d = \sum_{k=1}^{n}\rho D_k \frac{R_k}{y_k}\frac{\partial y_k}{\partial x_i}\frac{\partial y_k}{\partial x_i} > 0 \tag{12}$$

$(\dot{S}_{gen})_{ch}$: Chemical reaction volumetric entropy generation, $$(\dot{S}_{gen})_{ch} = \frac{\dot{\omega}}{T}\sum_{k=1}^{n}(\gamma'_k - \gamma''_k)\mu_k > 0, \tag{13}$$

4. Results and Discussion

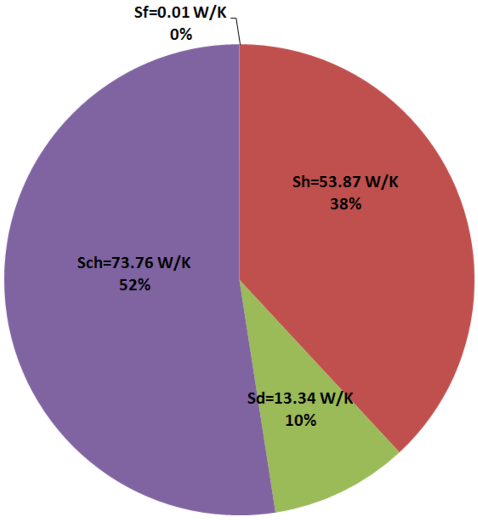

Figure 2. *Pie charts of entropy generation*

Figures 2 illustrates the pie chart of the entropy generation rate produced by the different mechanisms involved in the combustion process. The total generated entropy is about 140 W/K. Chemical reaction (52%) is the first producer of entropy. In the second order comes the heat conduction which is responsible of 38 %. Therefore, species diffusion transfers have moderate part (10%). The effect of viscosity friction is negligible regarding the generation of thermodynamic irreversibilities.

4.1 Effect of preheating air on entropy generation

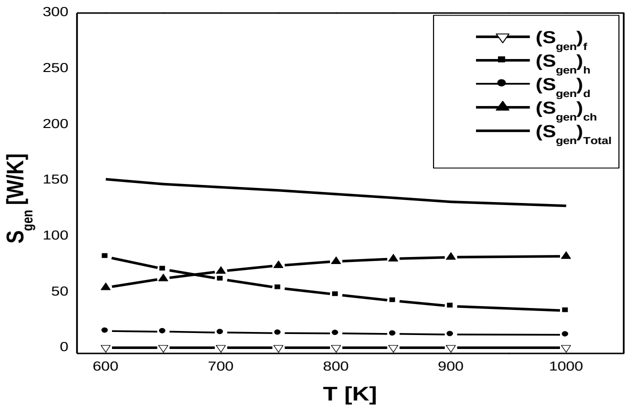

Figure 3. *Effect of preheating air on entropy generation.*

The variations of total entropy generation and also entropy generation associated to each mechanism versus air preheat temperatures are shown in Figure 3; the temperature of the inlet air supplied to the burner varies from 600 to 1000 K. The total entropy generation decreases with air temperature. Over the temperature range of 400 K, the generation of entropy is reduced approximately by 7%. That means every 10 K the entropy production decreases by 0.2%. This favorable effect of air temperature on reducing thermodynamic irreversibility of combustion process is attributed mainly to the role of heat conduction and species diffusion. This effect occurs in spite of the fact that preheating air has the adverse effect on the chemical reactions contribution. Increasing air temperature reduces the temperature difference between the reactants and the combustion products. This has the effect to soften the temperature gradients within the burner which lowers the thermodynamic irreversibility inherent to heat transfer at a finite temperature gradient.

4.2 Effect of air factor on entropy generation

In this section, the effect of air factor on the creation of thermodynamic irreversibilities in the combustion chamber is analyzed for each process of entropy generation contribution as shown in Figure 4. The air factor, λ, varies from 0.5 to 1.3. The combustors of gas turbines run always with air excess regime where the air factor is greater than 1(λ>1). The first result is that the total entropy generated by combustion process increases with increasing air factor, in deficit air as well as in excess air regimes. Entropy production due to heat conduction increases monotonously over all the range of air factor. The variation is more rapid in the air excess regime. The entropy generation caused by chemical reaction has two trends; at first, it increases in the air deficit regime (λ<1) and then decreases slowly in the air excess regime. The increasing entropy generation due to heat conduction and that due to the decreasing chemical reaction meet at air factor equals 1.3. Moreover, In air excess regime the burner is diluted by air, non combustible. Thus, an amount of heat combustion released in the burner is absorbed by non participating matter in the combustion reaction. This causes that the average level of flame temperature falls lower than its level obtained at stoichiometric fuel/air mixture. Among all the considered mechanisms, entropy generation due to heat conduction is more sensible versus air factor; it shows a more rapid variation because its dependency to temperature squared, in accordance with Equation (11).

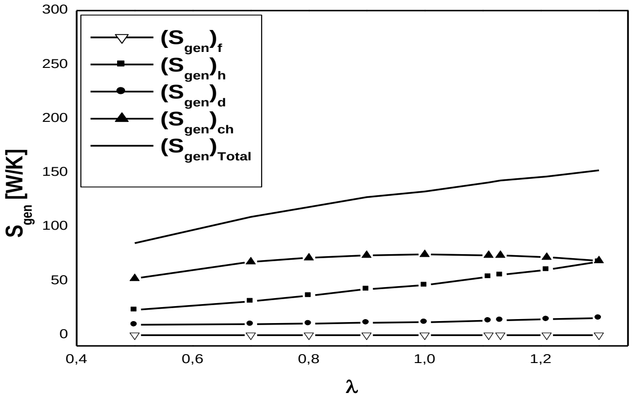

Figure 4. *Effect of air factor on entropy generation.*

Conclusion

The purpose of the paper is the assessing of the thermodynamic inefficiencies occurring during combustion processes. Through entropy generation analysis it is able to identify the role of every physical and chemical mechanism involved in generating thermodynamic irreversibilities. The analysis is based on the numerical simulation, by the software Fluent, of a typical combustion system. The case study consists of a turbulent diffusion flame burning in a co-axial jets cylindrical burner; a configuration representative of gas turbine combustors. At first, the results, in terms of velocity, temperature and species fields are compared to experimental reference data. Then, it appears that chemical reaction and heat transfer are the more important responsibles of thermodynamic irreversibilities; they are responsible, respectively, by 50% and 40% of entropy generation. The species diffusion has moderate role, around 10%, while the irreversibilities generated by viscous friction are negligible. Preheating inlet air has positive impact on the total thermodynamic irreversibilities associated to the combustion process by reducing the entropy generation due to heat transfer. Air excess has negative impact on the efficiency of combustion processes. It increases considerably the share and dominance of heat conduction in generating entropy.

Nomenclature

D	Coefficient of diffusion	ρ	Density
h	Enthalpy	ε	Dissipation of energy
k	Kinetic turbulent energy	ω	Arrhenius terms
L	Length of combustion chamber	λ	Thermal conductivity
p	Pressure	τ	Shear stress tensor
R	Constant of ideal gas		***Indice***
R, r	Radius	ch	Chemical reaction
S,s	Entropy	d	Species diffusion
T	Temperature	eff	Effective
U, u	Axial velocity	f	Viscosity friction
V	Velocity	gen	Generation
x	Cartesian coordinate	h	Thermal heat diffusion
y	Mass fraction of chemical species	i	Composite of Cartesian coordinate
	Greeks	j	Composite of Cartesian coordinate
α	Thermal Diffusivity	k	Chemical species
μ	Chemical potential, Viscosity	N	Number of chemical species

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