Numerical Simulation of Entropy Generation in Hydrogen Enriched Swirl Stabilized Combustion

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Abstract

Numerical simulations were conducted to estimate the change in entropy generation in swirl stabilized CH₄/air flame due to H₂ addition to the fuel stream. A finite volume computational model which solves the Reynolds Averaged Navier Stokes with the Re / k – ε turbulence model and laminar flamelet combustion model was used to compute the flow and energy fields of the flame. The numerical simulation was validated by comparing computed profiles of velocity and mixture fraction with established laser measurements of Sydney swirl burner. It was found that hydrogen enrichment results in an increase in the entropy generation rate of the flame. Such increase was attributed to the increase in heat transfer irreversibilities due to flame temperature rise.

Keywords: Entropy; Numerical analysis; Combustion model; PDF; Laminar flamelet model; Turbulence

1. Introduction

Hydrogen enrichment is a potential technique for improving natural gas combustion systems for power generation and industrial applications. The addition of hydrogen enables the combustion system to be operated at very lean conditions which improves the fuel economy and overall system efficiency [1, 2, 3]. However, the combustion of hydrogen causes significant temperature rise in some regions of the flame [4]. This might cause a reduction in the combustion system reversible work which could neutralize the fuel economy gains. The Gouy–Stodola theorem dictates that for a given thermodynamic system, the lost work is given by:

\[ W_{rev} - \dot{W} = T_a \dot{S}_{gen} \]  \hspace{1cm} (1)

where \( W_{rev} \) is the reversible (i.e. available) work, \( \dot{W} \) is the actual work, and \( \dot{S}_{gen} \) is the total entropy generated in the system. In general, entropy is generated due to numerous factors depending on the system properties such as heat transfer, viscous dissipation and chemical reaction. By considering

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the heat and mass irreversibilities in a thermodynamic system, the local entropy generation in a two
dimensional radial axisymmetric domain can be expressed in tensor notations as [5, 6]:

\[ \dot{S}_{gen} = \frac{k}{T} \left[ \left( \frac{\partial T}{\partial x} \right)^2 + \left( \frac{\partial T}{\partial r} \right)^2 \right] + \frac{\mu}{T} \gamma \] (2)

where the first and second terms on the RHS refer to entropy generation due to heat transfer \( \dot{S}_{ht} \) and
viscous dissipation \( \dot{S}_{\nu} \), respectively, and \( \gamma \) is the viscous dissipation term, expressed as:

\[ \gamma = 2 \left[ \left( \frac{\partial u}{\partial x} \right)^2 + \left( \frac{\partial v}{\partial r} \right)^2 + \frac{v}{r} \right] + \left( \frac{\partial u}{\partial r} + \frac{\partial v}{\partial x} \right)^2 + \left( \frac{\partial w}{\partial r} - \frac{w}{r} \right)^2 \] (3)

where \( u, v, \) and \( w \) are the axial, radial and swirl velocity components, respectively.

2. Mathematical Model and Numerical Details

The governing equations and procedures of the computational approach used herein are
explained in details in [7] and skipped here for brevity. The main difference in the mathematical
model in the present work is the use of the \( R_e / k - \varepsilon \) turbulence model proposed by Saqr et al [8] to
take into account the local anisotropy in swirling flows by modifying the \( \varepsilon \) equation in the standard
\( k - \varepsilon \) model. The model was validated for both reacting [9] and non-reacting [10, 11, 12] swirl
dominated flows. The laminar flamelet turbulent combustion was used in conjunction with a
presumed \( \beta \)-shaped probability density function to model the interaction turbulence and chemical
reaction. The GRI3.0 chemical reaction mechanism [13] was used to compute the chemical species.

In the present work attention is given to the changes in the local entropy generation rates due
to hydrogen enrichment of swirl-stabilized CH\(_4\)/air flame. ANSYS Fluent® was used to carry on
the computational work, and a compiled C# User Defined Function (UDF) subroutine was used to
compute the entropy generation based on equations (2, 3) and the reacting flow field variables.
Figure 1 shows a schematic of the Sydney burner [14, 15] and the 2D variable density numerical
grid used in the present work.

![Figure 1. Schematic of Sydney burner outlet plane and the computational domain which consisted of 9.3×10\(^4\) quadrilateral cells.](image)

3. Validation of the Numerical Simulation

For the purpose of validation, comparisons between the numerical solution of the reacting
flow field in SMH1 case [16] and experimental measurements are presented in figure 2. The numerical solution shows acceptable agreement with the LIF measurements of flame mixture
fraction in figure 2(a). For the velocity field predictions, the numerical solution shows substantially better agreement with the LDV measurements of axial velocity component as depicted in figure 2(b). The numerical solution has successfully predicted the central recirculation zone characterized by negative axial velocity, which proves the capability of the $R_e/k - \varepsilon$ turbulence model to model complex swirling flow with recirculation.

![Figure 2](image-url)

Figure 2. Comparison between numerical results (line) and LIF/LDV measurements (symbols) of (a) flame mixture fraction and (b) axial velocity on radial lines positioned 25 mm and 20 mm, from the burner exit plane respectively.

### 4.0 Effects of Hydrogen Addition on Entropy Generation

#### 4.1 Entropy Augmentation Number

The entropy augmentation number $N_{S,a}$ is the dimensionless ratio of local entropy generation in two specific cases $\left( \frac{\dot{S}_{\text{gen},1}}{\dot{S}_{\text{gen},1}} \right)$. In this context, $\dot{S}_{\text{gen},1}$ and $\dot{S}_{\text{gen},i}$ resemble the local entropy generation in CH$_4$/air flame (i.e. without H$_2$ enrichment) and in CH$_4$-H$_2$/air flame (i.e. with hydrogen enrichment), respectively. When $N_{S,a}$ is less than unity, it means that the addition of hydrogen resulted in a reduction of entropy, hence an enhancement of the system exergy. Figure 3 shows axial and radial profiles of $N_{S,a}$ for different hydrogen concentrations. The figure shows that the addition of H$_2$ causes substantial rise of $N_{S,a}$ in some locations of the flame, while in other locations it causes $N_{S,a}$ to decrease.

#### 4.2 Effects on Bejan Number

Bejan number is a dimensionless measure of the heat transfer irreversibility. It is computed as the ratio of heat transfer entropy generation $\dot{S}_{hi}$ to the total entropy generation $\dot{S}_{\text{gen}}$. Figure 4 shows the effect of hydrogen addition on local Bejan number on the axis of the flame. Bejan number exhibits sudden and sharp increase between 60 mm to 80 mm away from the burner exit plane due to hydrogen enrichment. This indicates the effect of temperature rise, which drives the heat transfer irreversibility.

### 5.0 Discussion and Conclusion

In the present paper, numerical simulations of the entropy generation in turbulent swirl flame have been conducted. In qualitative terms, it was found that the entropy generation rate
increases as a result of hydrogen enrichment. Such increase was detected as sharp rises in the entropy augmentation number. Then, a depiction of the Bejan number showed a corresponding rise of the heat transfer irreversibility, which is deemed to be the cause for the increase entropy generation rate. Future investigations should provide more detailed insights on the characteristics of entropy generation patterns and extend the analysis to cover a wider range of hydrogen concentration.

Figure 3. Profiles of entropy augmentation number ($N_{S,a}$) on (a) flame axis and (b) flame radius at axial distance of 55 mm.

Figure 4. Axial profile of Bejan number for different hydrogen enrichment ratios.

REFERENCES


