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Entropy generation in turbulent syngas counter-flow diffusion flames

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ABSTRACT

Efficiency is one of the major objectives when designing energy systems. Irreversibilities of combustion processes can be characterized by analyzing entropy generation which is proportional to exergy destruction. In this paper, entropy generation is investigated in turbulent non-premixed counter-flow syngas flames at a high strain rate over a wide range of hydrogen percentage (H_2/CO molar fraction from 0.4 to 2.0). The aim is to define the most efficient syngas composition to reduce irreversibilities. Irreversibilities involved in NO formation process are also examined. RANS (Reynolds Averaged Navier Stokes) technique including k-ε turbulence model is used for the flow field estimation. Flame structure is calculated using SLFM (Steady Laminar Flamelet Model) and EPFM (Eulerian Particle Flamelet Model) is applied for NO_x predictions. Total entropy generation rate accounts for chemical, heat conduction, mixing and viscous effects. Computational results show that the total volumetric entropy generation decreases with H_2 enrichment as well as its different contributing effects. Chemical effect is dominant, followed by heat conduction and mixing effects. Viscous effect is negligible. The maximum of both thermal and prompt NO formation routes are influenced by the three main entropy generation modes, with the predominance of the chemical effect. At high strain rates, H_2-rich syngas flames are efficient in regards to irreversibilities and NO emissions reduction.

Introduction

Modern societies are heavily dependent on energy which is mainly supplied using fossil fuels. The limited fossil fuel resources combined to the need for reducing pollutant emissions have increased the interest for hydrogen blended fuels like syngas. From combustion viewpoint, hydrogen is probably the nearest to an ideal fuel [1]. It has wide burning limits, easy ignition and high flame speed. When burning, it does not produce CO and CO_2 or even soot. In spite of formidable design and logistics problems, hydrogen is worthy of consideration as an alternative fuel [1].

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Hydrogen and syngas have great potential in addressing three major challenges in energy area: to supply clean fuels in order to fulfill the increasing energy requirements, to increase the efficiency of energy utilization and to reduce pollutant emissions [2].

Syngas is a hydrogen-rich renewable fuel mainly composed of hydrogen and carbon monoxide. The combustion of this blended fuel is an important component of the IGCC (Integrated Gasification Combined Cycle) concept. The use of syngas as a fuel meets significant benefits in terms of both reducing pollutant emissions and energy economy.

Efficient use of energy is one of the major objectives in designing modern combustion chambers. Efficiency of a process can be assessed using the irreversibilities generated. Thus, reducing entropy will result in a more efficient design of the system.

The last few decades, methods based on entropy generation minimization have gained a great interest.

Bejan [3] published the pioneering work on entropy generation minimization in thermal systems. He analyzed the phenomena behind entropy generation in applied thermal engineering. In a second study [4], he investigated entropy generation in several sectors of thermal engineering. Later on, several studies have been devoted to the entropy generation. For example, Mahmud et al. [5,6] applied the second thermodynamics law analysis to study heat transfer problems. They analyzed second law characteristics of heat transfer and fluid flow due to forced convection of steady-laminar flow of incompressible fluid inside channel with circular cross-section, channel made of two parallel plates and circular annulus. They established entropy generation profiles and heat transfer irreversibility characteristics for each case. They found that the expression of entropy generation has three main parts. The first part is related to axial conduction. The second and third parts are related to heat transfer and fluid friction respectively.

Many similar studies have been carried out to analyze the entropy generation due to heat transfer and flow friction in ducts [7–12].

For combustion processes, entropy generation has been also evaluated in many studies including premixed and diffusion flames. The purpose was to identify the predominant irreversibilities and the effect of some parameters like hydrogen addition and preheating [13–15]. Teng et al. [16] provided an entropy generation equation for multicomponent laminar hydrogen flames. They suggested that species diffusion induces a diffusive-viscous effect which could contribute significantly to entropy generation in multicomponent fluid systems.

Nishida et al. [17] also studied entropy generation and exergy loss during combustion. The effects of fuels, equivalence ratio and inlet fluid temperature on local entropy generation were evaluated for both hydrogen and methane premixed and diffusion flames. It was found that chemical reaction is the major process for entropy generation and exergy loss in premixed flames. Its contribution in the methane fueled flame is less than in the hydrogen fueled flame. Decreasing the equivalence ratio and the inlet fluid temperature increases the exergy loss in premixed flames. For diffusion flames, the major source of entropy is heat conduction.

Okong'o and Bellan [18,19] considered an *n*-heptane/nitrogen 3D supercritical mixing layer and analyzed entropy generation effects by Direct Numerical Simulation (DNS). Their results showed that the average entropy production is dominated by the viscous terms at all stages of the evolution.

Yapici et al. [20] presented a numerical study of equivalence ratio and oxygen fraction effects on local entropy generation in a turbulent premixed methane-air burner. Simulation was performed to calculate the volumetric entropy generation rate and some other thermodynamic parameters. Equivalence ratio was taken from 0.5 to 1.0 and oxygen percentage from 10 to 30%. The results showed that the increase of equivalence ratio significantly reduces the reaction rate levels. Moreover, the average temperature in the combustion chamber increases with increasing oxygen fraction and equivalence ratio. The increase of oxygen fraction reduces the volumetric local entropy generation rate.

Yapici et al. [21] carried out a numerical study on local entropy generation in a burner fueled with hydrogen and various hydrocarbons. The fuel mass rates were adjusted to provide the same heat transfer rate to the combustion chamber. Fluent software was used to numerically solve the combustion equations. Furthermore, a computer program was developed to numerically calculate the volumetric entropy generation rate distributions and the other thermodynamic parameters, i.e. the temperature, the rate of total irreversibility and the rate of exergy transfer accompanying energy transfers, on the basis of flow and temperature fields provided by Fluent. The results showed that the increase of the equivalence ratio from 0.5 to 1.0 decreases the volumetric local entropy generation rates about 4% and increases the Merit numbers about 16%.

Daw et al. [22] considered an isobaric combustion process that utilizes controlled preheating to enhance near-equilibrium combustion of hydrogen flames. They proved that it is theoretically possible to eliminate the majority of irreversibilities by preheating the hydrogen and the air in a counter-flow heat exchanger with recycled flue gas.

Som and Datta [23] presented a comprehensive review pertaining to fundamental studies on thermodynamic irreversibility and exergy analysis in the processes of gaseous, liquid and solid fuel combustion. They recognized that, in almost all situations, the major source of irreversibilities is the internal thermal energy exchange associated with high-temperature gradients caused by heat release in combustion reactions. The optimum operating condition in this context can be determined from parametric studies on combustion irreversibilities with operating parameters in different types of flames.

Briones et al. [15] analyzed the entropy generation in laminar hydrogen-enriched methane-air propagating triple flame. Their study was based on computing the entropy generation terms in a transient reacting flow field. They found that H_2 addition to methane increases entropy generation since it enhances heat conduction and chemical reactivity. The contribution of chemistry and heat transfer to entropy generation depends on the flame configuration rather than the fuel being burned.

Chen et al. [24] investigated entropy generation in hydrogen enriched ultra-lean counter-flow methane–air

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