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# A numerical investigation of structure and emissions of oxygen-enriched syngas flame in counter-flow configuration



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#### ABSTRACT

The aim of the present study is to investigate the enhancement of syngas combustion using the promising oxygen-enrichment technology, with a particular attention on optimal operating conditions in regard to  $NO_x$  emissions. For this purpose, a numerical study is conducted on a syngas counter-flow diffusion flame, using air enriched with oxygen as the oxidizer. The oxygen concentration ranges from 21% to 30% by volume. Two syngas compositions are considered with  $H_2/CO$  rates equal to 0.25 and 4, respectively. Flame structure is characterized by solving flamelet equations with the consideration of radiation. The chemical reaction mechanism used is GRI 3.0. Computational results showed that oxygen addition increases the flame temperature and intensifies the radiative heat transfer. It also considerably extends flammability limits allowing stable flames at high values of the scalar dissipation rates and for lean syngas composition.  $NO_x$  formation is substantially increased with oxygen increment, and Zeldovich mechanism is found to be the main route of  $NO_x$  formation.  $H_2$ -lean syngas flames produce less  $NO_x$  at low scalar dissipation while  $H_2$ -rich syngas flames  $NO_x$  emissions are low at high scalar dissipation rates.

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#### Introduction

Conventional fuels are expected to be progressively replaced by cleaner energy sources, among which, hydrogen-rich fuels such as syngas, are due to become the most important alternative ones.

The use of syngas is of increasing interest, particularly for electricity production and as a component of the Integrated Gasification Combined Cycle concept (IGCC).

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The composition of syngas is strongly dependent on the fuel source and processing technique [1]. Syngas may have wide variations of  $H_2$ /CO ratios. Hence, combustion properties such as flammability limits and flame temperature will be accordingly variable. In addition, syngas, as many alternative fuels, has lower calorific value than conventional fuels such as methane. According to McLean et al. [2], a syngas with a  $H_2$ /CO ratio equal to 0.5 has a Low Heating Value (LHV) of 10.5 MJ/kg, while methane has a LHV of 50 MJ/kg [3].

Oxygen-Enriched Combustion (OEC) has been advanced as cost effective option to improve combustion process (stability and reactivity) [4]. Oxygen-enriched combustion, also known as oxygen-enhanced combustion, uses oxidizers with oxygen concentrations higher than that in air (21% by volume). It is applied since many years, in different industries, such as cement and glass factories, waste incineration and steel smelting. OEC has received, by the past, little attention from the academic combustion community, due to safety considerations and high costs of oxygen production [4]. Recent investigations showed that increasing oxygen concentration in the oxidizer induces several benefits including higher flame temperatures, rising productivity and significant reduction in fuel consumption [5,6]. Moreover, recent increasingly strict emissions regulations and costs reduction of oxygen production have revived the interest of researchers to oxygenenhanced combustion.

Tan et al. [7] carried out an experimental study on the effects of oxygen enrichment in air and CO<sub>2</sub> atmospheres in the case of methane flame using a vertical combustor. The O2 concentration was set to 28% in both cases. Very high levels of NO<sub>x</sub> were obtained in O<sub>2</sub> enriched air combustion due to higher flame temperatures while nearly no NO<sub>x</sub> emissions were observed in  $O_2/CO_2$  combustion due to the absence of  $N_2$ in the feed air. Cheng et al. [8] investigated by both numerical simulation and optical measurements the structure of a planar oxygen-enriched methane counter-flow flame. They particularly focused their attention on the effects of stretch and oxidizer oxygen concentration. They found that, for a given value of stretch, flame temperature increased significantly with oxygen concentration. Moreover, they observed that oxygen enrichment considerably enhanced extinction limits. Chen and Axelbaum RL [9] conducted an experimental and a numerical study to examine the effects of oxygenenrichment and fuel dilution on flame extinction. They considered a counter-flow flame configuration and four different fuels: methane, ethane, ethylene and propane. The range of oxygen mass fraction variation was from 0.233 to 1.0. Results indicated that an appropriate adjustment of oxidizer oxygen and fuel concentrations give improved extinction characteristics. In other words, an optimal oxygenenrichment, combined with fuel dilution, leads to strong flames [9]. A numerical study of CH<sub>4</sub>/air and CH<sub>4</sub>/O<sub>2</sub> counterflow laminar flames was performed by Urzica and Gutheil [10] using a detailed chemical reaction mechanism. The laminar CH<sub>4</sub>/O<sub>2</sub> flame was studied under pressures ranging from 0.1 MPa to 2 MPa. It was shown that maximum flame temperature increased significantly with oxygen concentration in the oxidizer. The same trend was observed for radicals CO. O and OH. Furthermore, comparison between CH<sub>4</sub>/air and CH<sub>4</sub>/ O<sub>2</sub> flames at strain rate near extinction revealed that flame thickness decreased considerably when oxygen oxidizer content increased. Global effects of oxygen-enhancement on radiative heat flux characteristics of methane non-premixed oxyfuel flames were examined experimentally by Ditaranto and Oppelt [11]. The oxidizer oxygen concentrations were varied from 35% to 70%, and  $CO_2$  was used as a diluent. The measurements performed along the flame axis showed that the distribution of radiative heat flux and the flame length became shorter when the oxygen concentration increased. Moreover, the peak of radiated heat flux increased with oxygen concentration [11]. Furthermore, the intensity of visible spectra of these flames was more important with oxygen enrichment. Joo et al. [12] performed a numerical and an experimental study of the structures of laminar diffusion methane/oxygen and methane/air flames under a wide range of operating pressures (from 1 atm to 60 atm). The authors observed that, as the pressure increased, the visible flame height of the methane/oxygen flames decreased, while the visible flame height of methane/air flames remained constant. The comparison of soot production, for different pressures, showed that maximum soot fraction produced by methane/ air flames was considerably higher than in methane/oxygen flames [12].

Yepes et al. [13] analyzed experimentally and numerically the laminar burning velocities of a syngas mixture containing 20% H<sub>2</sub>, 20% CO and 60% N<sub>2</sub> using oxygen enriched air with enrichment levels varying from 21% to 35% by volume. They found that oxygen rise in the combustion air increased the laminar burning velocity of the syngas mixture, leading to an intensification of the reaction rate.

The literature on oxygen-enhanced diffusion flames is abundant, but only few studies are devoted to syngas oxygenenhanced flames characteristics.

The aim of this study is to examine numerically the impact of oxygen enrichment on the structure and emissions of syngas flame in counter-flow configuration. The calculations are conducted over a large range of scalar dissipation rates (from near equilibrium to near extinction) for oxygen concentration ranging from 21% to 30% by volume, and for two

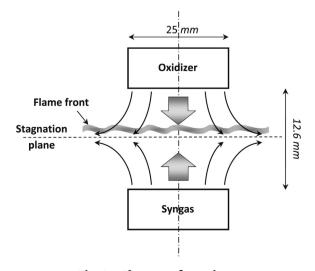


Fig. 1 – Flame configuration.

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