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Structure and reaction zones of hydrogen – Carbon-monoxide laminar jet diffusion flames

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ABSTRACT

In this study, experimental and numerical investigations of laminar jet diffusion flames using carbon-monoxide – hydrogen mixtures are carried out. Using a simple experimental setup, high definition direct flame photographs and shadowgraphs are captured, and radial temperature profiles at two axial locations are measured. Numerical simulations of carbon-monoxide – hydrogen jet diffusion flames have been carried out using a comprehensive computational model, along with simplified detailed chemical kinetics mechanism having 14 species and 38 reactions, and an optically thin approximation based radiation sub-model. Validation of the numerical model is carried out by comparing the measured and predicted temperature profiles, and experimental shadowgraph images with second derivative of the predicted density field. Results from the numerical simulations provide insights to the structures, species and thermal fields of flames for varying hydrogen content in the fuel mixture. It is observed that the axial extent of the maximum temperature zone tends to move towards the burner exit as the percentage of hydrogen in the fuel increases. It is also observed that the maximum mass fraction of carbon-dioxide decreases and those of OH and water vapour increase with increasing percentage of hydrogen in the fuel. Radial distributions of important species are presented for varying hydrogen content in the fuel mixture, which clearly illustrate the structure of the flame. Radial profiles of net reaction rates of major species and net rates of few important reactions are presented. As hydrogen is added, the reaction zone moves out in the radial direction, increasing the radius of the flame.

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Introduction

The increased usage of petrochemical energy and its demand, as well as, the increasing concerns of green-house gases emissions have given rise to the research of alternative fuels. Hydrogen or hydrogen blended fuel has become an attractive

option to reduce the fossil fuel consumption and carbon emissions. Syngas, also known as synthetic gas, which consists of CO and H₂ as the main fuel components, can be obtained from the gasification of coal, biomass, and refinery residual and even municipal waste. Thus, instead of using hydrogen, it is more practical and economical to use syngas directly. However, one of the particular concerns in this

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process is the variation in the composition of the syngas because of its source, and more particularly, the variation in the ratio of CO and H₂. Therefore, it is necessary to study the effect of variation in the composition of syngas. The non-fuel components in syngas such as N₂ and CO₂ can be reduced by using oxygen rich oxidizer for gasification and using available sequestration process. Therefore, investigation of burning characteristics of CO and H₂ mixtures of varying compositions, in the jet diffusion flame mode, which is the simplest combustion mode due to the simplicity of the burner setup, using parameters such as flame length, thermal plume width, temperature and luminosity, forms the primary focus of the present study.

A considerable amount of research works on hydrogen addition to fuels, on combustion of syngas or CO/H₂ fuel mixtures, along with associated emissions, are available in literature. Investigations of the burning characteristics of premixed synthetic gas–air mixtures have been performed to estimate the laminar flame speed (Mclean et al. [1]) and to understand its ignition and extinction characteristics (Fotache et al. [2]). The combustion characteristics of syngas are quite different from pure hydrogen or pure hydrocarbon gases. Davis et al. [3] conducted experiments as well as numerical simulations to study the dynamics and structure of lean CH₄/air flames in the presence of species such as H₂, CO, and CO₂. The main focus was on the effect of H₂ addition and the strain rate. They concluded that the fundamental flammability limits and the laminar flame speed may not be a good measure for the enrichment of the combustion intensity, specifically when it is achieved through highly diffusive additives, such as hydrogen. The effects of fluid mechanics, as manifested by the induced strain rate, must also be considered. Vagelopoupos et al. [4] conducted studies mainly for stretch corrected measurements on laminar flame speeds in counter-flow flames. Drake and Blint [5] used an opposed flame configuration to investigate the effect of flame stretch on the production of NO using CO/H₂/N₂ fuels. They concluded that with an increment in flame stretch the NO concentration decreased dramatically. Measurements and modelling of NO in premixed CO/H₂/CH₄/air flames at high pressures was reported by Charlston et al. [6]. They concluded that NO concentrations were increasing with increase in both pressure and equivalence ratio. Giles et al. [7] investigated NO_x emission characteristics of syngas diffusion flames with air stream dilution using counter-flow flame configuration. They selected two types of syngas mixtures having equal molar percentages of CO and H₂, and mixed it with three diluents, N₂, H₂O and CO₂ along with air. They concluded that a reduction in both flame temperature and the concentration of CH radical occurs, which decreases thermal and prompt NO. Som et al. [8] studied the combustion and NO_x characteristics of syngas fuel with varying composition, pressure and strain rates. They had established stable non-premixed and partially premixed counter-flow flames and studied them both experimentally and numerically. Further, the effect of syngas addition on NO formation in strained methane/air diffusion flames was investigated by Guo and Neil [9]. Ding et al. [10] numerically investigated the extinction limits and emission characteristics of dry syngas with equimolar CO/H₂, moist syngas (with 20% H₂O) and impure syngas (with 5% CH₄) at

lean premixed combustion conditions. Results showed that NO formation for impure syngas was completed through a dominant NNH route. Flames with richer hydrogen content and higher flame temperature consumed more nitrogen through thermal, prompt and intermediate N₂O routes. They also concluded that in different compositions of syngas, higher CO concentration leads to higher NO emissions.

Karbazi and Wierzbza [11] studied the burning of a mixture of methane-hydrogen with a co-flow oxygen stream both experimentally and analytically. A higher stability was observed in methane jet diffusion flame when hydrogen was added either to the fuel side or to the surrounding oxidizer stream. Karim et al. [12] observed that an addition of hydrogen to methane fuelled spark ignition engine enhances the thermal efficiency and reduces the emission levels. A co-flow diffusion flame of hydrogen-hydrocarbon fuel was used by Choudhuri and Gollahalli [13] to investigate the flame structure and related characteristics. They reported that, an increase in the flame length and flame luminosity occurred with an increase in the volumetric content of natural gas or propane in the fuel mixture. They also observed a reduction in NO and NO_x emission, as well as an increase in the CO emission. Choudhuri and Gollahalli [14] concluded that the fuels with higher hydrogen content burn faster and has a shorter flame length. Choudhuri and Gollahalli [15] investigated the flame temperature and intermediate radical concentrations of OH, O, H, and CH in different mixtures of hydrogen-natural gas fuelled diffusion flames at a burner exit Reynolds number of 150. Hu et al. [16] studied various characteristics of methane-hydrogen-air flames both experimentally and numerically. They concluded that there was an enhancement in the chemical reaction rate with H₂ addition. This enhancement was attributed to the increase in the mole fractions of H, O and OH radicals. The characteristics of hydrogen jet diffusion flames, to examine the fundamentals of hydrogen related fires, were investigated by Schefer et al. [17]. They concluded that the hydrogen jet flame height was proportional to the nozzle diameter and the flow rate of the fuel. Cheng et al. [18,19] investigated the burning of mixture of hydrogen and hydrocarbon fuels in counter-flow configuration. They examined the structure of lean hydrocarbon and counter-flowing premixed hydrogen flames both experimentally and numerically. The outcome of their numerical simulations of premixed hydrocarbon and hydrogen flames was about an optimal chemical reaction mechanism for the interaction of premixed hydrocarbon and hydrogen flames. Recently, Alex et al. [20] have investigated the structures and reaction zones of methane–hydrogen laminar jet diffusion flames using a comprehensive numerical model.

It is quite evident from the previous studies on CO–H₂ combustion that, most of the studies are either on premixed or counter-flow diffusion configurations. Basic structure and detailed reaction zones of CO–H₂ jet diffusion flames, using adequate elementary reaction mechanisms, have not been reported in detail. These gaps in the literature form the motivation of the current work. In this study, the effects of hydrogen addition on temperature and species distributions in laminar jet diffusion flames are analyzed. Further, the effects of hydrogen content in the fuel blend on the flame structure and reaction zones are studied in detail.

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