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Effects of content of hydrogen on the characteristics of co-flow laminar diffusion flame of hydrogen/nitrogen mixture in various flow conditions

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ABSTRACT

Effect of content of hydrogen (H_2) in fuel stream, mole fraction of H_2 (X_{H_2}) in fuel composition, and velocity of fuel and co-flow air (V_{avg}) on the flame characteristics of a co-flow H_2/N_2 laminar diffusion flame is investigated in this paper. Co-flow burner of Toro et al. [1] is used as a model geometry in which the governing conservation transport equations for mass, momentum, energy, and species are numerically solved in a segregated manner with finite rate chemistry. GRI3 reaction mechanisms are selected along with the weight sum of grey gas radiation (WSGG) and Warnatz thermo-diffusion models. Reliability of the newly generated CFD (computational fluid dynamics) model is initially examined and validated with the experimental results of Toro et al. [1]. Then, the method of investigation is focused on a total of 12 flames with X_{H_2} varying between 0.25 and 1, and V_{avg} between 0.25 and 1 ms^{-1}. Increase of flame size, flame temperature, chemistry heat release, and NOx emission formation resulted are affected by the escalation of either X_{H_2} or V_{avg}. Significant effect on the flame temperature and NOx emission are obtained from a higher X_{H_2} in fuel whereas the flame size and heat release are the result of increasing V_{avg}. Along with this finding, the role of N_2 and its higher content reducing the flame temperature and NOx emission are presented.

Introduction

The demand for energy, which is increasing significantly, and the concern of environmental issues encourage the research and development in the various sectors of clean and sustainable energy. Among them, one of the attractive options is hydrogen (H_2) mixture fuel which can be produced by several methods (such as gasification, carbonization, steam reforming, and thermolysis), and also from flexible feedstocks (such as coal, wood and biomass). Research and development relating to this fuel, which is considered to be environmentally friendly and sustainable, has been focused on both the production techniques and the possibility of replacing the conventional carbon fuel used in various combustion systems. Since different methods are employed for the production of H_2 mixture fuel, the composition of H_2 mixture fuel is varied and depends strongly on the production technique and feedstock. Fuel composition could be a mixture of H_2, which is a major fuel component, with other species such as carbon monoxide

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Nomenclature

Uppercase letters

C_v	Contribution to the molar specific heat of each specie
$D_{i,t}$	Thermal diffusion coefficient
D_m	Molecular diffusivity of multi component gases
$D_{i,m}$	Binary diffusion of component *i* and *m*
$F_{k,j}$	Diffusive flux component
$\vec{J}$	Diffusive flux
K_k	Absorption coefficient of each grey gases
S_h	Heat due to chemical reaction and radiation
K	Total number of grey gases
M	Molecular weight
S	Optical path length
T	Temperature
T^*	Reduced temperature
V	Velocity of fuel and air
X	Mole fraction
Y	Mass fraction

Greek letters

ρ	Fluid density
σ	Collision diameter
$\bar{\bar{\tau}}$	Viscous stress tensor
μ	Molecular viscosity
ω	Production rate of each specie
Ω	Collision integral

Lowercase letters

a_k	Weight factor
g	Gravitational acceleration
h	Specific enthalpy
k	Thermal conductivity coefficient
p	Pressure r Radial coordinate
v	Velocity
$\dot{v}$	Volume flow rate

Subscripts

i	component i
j	Specie j
k	Specie k
m	Multi component or component m
x	Component in axial direction
r	Component in radial direction
tran	Translation
rot	Rotation
vib	Vibration
avg	Average
max	maximum

Abbreviations

CVODE	A package written in C for solving differential equation
DARSCFD	Digital analysis of reaction systems

(CO), carbon dioxide (CO_2), nitrogen (N_2), and methane (CH_4) at different percentage of volume or mass. This variation thus points to the necessity of understanding the microscopic processes governing the combustion characteristics of this fuel.

Diffusion flame is selected as a source of heat energy in several applications and, characteristics of this flame were presented in the literature. A summary of the papers relating to the flame characteristics of H_2 mixture and H_2/hydrocarbon fuel is presented in Table 1. In those papers, the effect of the content of H_2 in fuel composition on the flame characteristics was examined through diffusion flame generated by a counter-flow or co-flow configuration at various strain rates and flow regimes. A large number of research papers paid attention to the turbulent flame whereas the work focusing on the laminar flame is limited. Flame structure, temperature and species profile were studied by the numerical and experimental methods. And the topics of interest could be categorised as: (i) the effect of adding H_2 content to hydrocarbon fuel, (ii) the effect of H_2 content on the flame characteristics of H_2 mixture fuel, and (iii) the effect of chemistry reaction mechanisms of H_2 mixture fuel.

In the first category, increasing stability and reducing CO emission were expected to be the result of adding H_2 content into the composition of hydrocarbon fuel since a lower content of hydrocarbon was supplied into combustion. This expectation was achieved in Ref. [2–5] where the flames of H_2/hydrocarbon e.g. H_2/C_3H_8, H_2/CH_4, and H_2/natural gas with different X_{H_2} were studies. Nevertheless, the addition of H_2 content also affected the characteristics of flame strongly. For example, the flame dimension was reduced whereas the NOx and soot emission formulations resulted at a higher rate than a conventional hydrocarbon fuel. Moreover, the faster burning rate along with the higher flame temperature due to the role of H_2 in combustion was the cause of this effect.

With regard to the H_2 mixture fuel, the role and effect of the H_2 content on the diffusion flame characteristics were studied in several research papers. Attention was paid to the flame structure, temperature, and species distribution profiles. Syngas (H_2/CO) and syngas with the dilution of N_2, CO_2, and H_2O diffusion flame generated by a counter-flow burner were also studied in Refs. [6] and [7], while the syngas and the H_2/N_2 turbulent flame formulated by a co-flow burner were examined in Ref. [8]. A similar result was obtained from both the burner configurations. In terms of the temperature of both the syngas and H_2/N_2 flames, fuel containing a higher content of H_2 formulated a higher flame temperature. Additionally, the flame dimension was found to be larger and more affected by the content of H_2 than for syngas and H_2/N_2, which is in contrast to an enrich CO flame.

The chemical reaction mechanisms capable of computing combustion of H_2 mixture fuel have been studied and presented in a number of research papers. Majority of them focused on the combustion of syngas (H_2/CO). However, the mechanisms presented have the potential to predict the reactions of a H_2 mixture fuel since the various species were taken into account [9] and [10]. In addition, a review and comparison of the various reaction mechanisms have been presented in Ref. [11] with the aim of finding the most suitable chemical mechanism compositions for predicting and explaining the syngas combustion. A total of 16 recent mechanisms such as GRI3 [12], Kéromnès-2013 [13], Davis-2005 [14], Li-2007 [15], Burk-2012 [16] and NUIG-NGM-2010 [17] can also provide a good prediction of computational result with experiment; however, the level of accuracy of each