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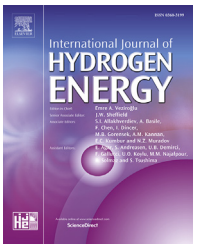

Kinetic simulation of flameless burners with methane/hydrogen blended fuel: Effects of molecular diffusion and Schmidt number☆

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ABSTRACT

The newly developed concept of MILD combustion has paved the way through achievement of high thermal efficiencies with low levels of pollutants and greenhouse gases. High fidelity numerical models play key role in design and optimization of these burners. The present research aims to assess the effect of molecular diffusion and deviations in the amount of different species Schmidt number on the precision of the model. To this end, a previously investigated MILD burner is opted as case-study. From the results it is evident that in contrast to conventional combustion regimes problems, the impact of the often-neglected laminar diffusion is comparable to turbulent diffusion. On the other hand, consideration of molecular diffusion in the species transport equation significantly improves the model accuracy only if proper Schmidt number for species are considered. Suitable Sutherland coefficients and Schmidt numbers for each species are found based on relevant data in the literature and reported.

Introduction

Today, combustion of fossil fuels has antagonistic impacts on human living. While, it enhances about 80% of the world energy demand, the pollutant species and greenhouse gases (GHG hereafter) emitted from the flames are proved to be associated with several threads to human health and environment. Carbon dioxide contributes 77% of the GHG emissions with combustion accounting for 27%, making it a major contributor to global climate change. This issue, has fired the enthusiasm of researchers and engineers in new combustion technologies. In this framework, precise numerical models are indispensable to meet the rapid responses required of regulatory agenda with feasible cost.

Preheating the reactants by the hot flue gases is proved to be a promising method to improve the combustion efficiency. This method has roots in the concept of "large excess enthalpy combustion" which was introduced in the early 1970s [1,2] and has paved the way for introduction of moderate or intense

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Nomenclature

A	Sutherland relation parameter
C	Diffusion coefficient
h	Enthalpy
k	Turbulent kinetic energy
p	Static pressure
R	Reynolds stress tensor
S	Source term for species conservation equation
Sc	Schmidt number
t	Time
T	Temperature
u	Velocity
Y	Mass fraction

Greek letters

ε	Turbulent dissipation rate
μ	Dynamic (absolute) viscosity
ρ	Density
ω	Source term for species conservation equation

Subscripts and superscripts

i, j, k	Pertinent to coordinate system
l	Pertinent to lth specie
M	Pertinent to molecular
S	Pertinent to sutherland
T	Pertinent to turbulent

low-oxygen dilution (MILD hereafter) combustion also known as flameless combustion [3]. Nevertheless, considering its different characteristics, this regime is known with several other names, some of which are: High Temperature Air Combustion or HiTAC [4], Colorless Combustion [5], invisible flame [6], High Temperature Combustion Technology or HiCOT [3], and the green flame [7]. Beside high efficiency, excellent combustion stability, uniform temperature distribution and extremely low emissions of NOx [8,9] are known as other beneficial features to flameless combustion regime. This last feature made researches i.e., Mardani and Tabejamaat [10], Li et al. [11] and Galletti et al. [12], to perform experimental and kinetic studies on formation of nitrogen oxides.

With the oxygen dilution range of 3–13% and reactant temperature always higher than the auto ignition temperature, the flameless combustion characteristics differ greatly from normal combustion. Therefore, many researches have addressed characteristics of flameless burners. Aminian et al. [13] numerically investigated the structure of a flameless burner with three different fractions of oxygen in hot coflow air jet using steady state Reynolds-Averaged Navier-Stokes (RANS hereafter) approach coupled with the Eddy Dissipation Concept (EDC hereafter) [14–16] for treating chemistry-turbulence interaction. Four variants of the well-known $k-\varepsilon$ model, i.e., standard, modified, realizable and RNG, and three different reduced kinetic schemes, i.e., DRM-19, DRM-22 and KEE-58, were utilized. The results indicate better performance of the KEE-58 mechanism in comparison with other schemes. Nevertheless, a large over-prediction of temperature and chemical species, except for oxygen molecule, at downstream was assessed for all flames, particularly for the flame with the lowest amount of oxygen in the hot coflow stream, i.e., 3%. It was also indicated that localized extinction did not contribute in the overprediction, which was thought to be due to turbulence-chemistry interaction model employed, whose importance was previously emphasized by Parente et al. [17] and Mardani et al. [18]. Also, for MILD regime, higher residence time in the fine structures for MILD combustion was indicated camparing with conventional combustion. Before that, Aminian et al. [19] and Frassoldati et al. [20] have shown the importance of implementing boundary conditions in utilizing coupled modified $k-\varepsilon$ model and EDC with reduced chemical mechanisms to simulate the MILD burners using CH_4-H_2 blends. In addition, MILD burners whose fuel jet are enriched with hydrogen have been subject of numerous other investigations. Mardani and Tabejamaat [21] studied the influence of hydrogen amount used to enrich methane fuel for burning under MILD conditions. In this research, which have employed modified $k-\varepsilon$ model coupled with EDC, improvements in mixing, and increase in mixture ignitability, flame entrainment, reaction intensities and rate of heat release with increase in the amount of hydrogen was assessed. Later, Afarin and Tabejamaat [22] utilized Large Eddy Simulation (LES) to study the effect of hydrogen enrichment and to show the increase in flame thickness and decrease in hydroxide oscillations in presence of hydrogen. In addition, in other research [23] they used LES to investigate the impact of fuel inlet turbulence intensity on the MILD flame structure and weakening of the combustion zone. In these two researches, the turbulence-chemistry interactions were modelled under the light of utilizing a modified version of EDC which is commonly referred as Partially Stirred Reactor (PaSR hereafter) model [24]. It is worth considering that turbulent transport, rooted in velocity fluctuations that act to efficiently transport momentum, heat, and species concentration, is significantly more effective that molecular diffusion [25]. The turbulence high rate of diffusivity caused molecular diffusion be neglected in many researches that deal with conventional turbulent combustion problems. Similarly, in the researches mentioned above, only the turbulent diffusion is considered. The effect of molecular diffusion was compared with that of turbulent diffusion in the flameless combustion regime by Mardani et al. [26] and the outcomes of using two different methodologies for considering molecular diffusion, i.e., bimolecular and multicomponent, were assessed. This research proved the importance of considering molecular diffusion taking the special characteristics of this regime into account.

The present research aims to investigate the influence of molecular diffusion on the validity of numerical simulation results for a burner working at flameless conditions for different inlet configurations. To accomplish this, a flameless burner is simulated with two different strategies; in the first strategy, the molecular diffusion is neglected, whereas in the second strategy, it is taken into account in the formulation. Also, two different methodologies are used for implementing the latter strategy to observe the impact of considering variations in Schmidt number of each specie on the fidelity of the results. The results are compared with each other and their deviation from the experimental observations, which has been reported by Dally et al. [27], are also assessed. Sutherland

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