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# Effect of different turbulence models on combustion and emission characteristics of hydrogen/air flames

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ABSTRACT

This paper aims to present modeling results of hydrogen/air combustion in a micro-cylindrical combustor. Modeling studies were carried out with different turbulence models to evaluate performance of these models in micro combustion simulations by using a commercially available computational fluid dynamics code. Turbulence models implemented in this study are Standard $k$-$\varepsilon$, Renormalization Group $k$-$\varepsilon$, Realizable $k$-$\varepsilon$, and Reynolds Stress Transport. A three-dimensional micro combustor model was built to investigate impact of various turbulence models on combustion and emission behavior of studied hydrogen/air flames. Performance evaluation of these models was executed by examining combustor outer wall temperature distribution; combustor centerline temperature, velocity, pressure, species and $NO_x$ profiles. Combustion reaction scheme with 9 species and 19 steps was modeled using Eddy Dissipation Concept model. Results obtained from this study were validated with published experimental data. Numerical results showed that two equation turbulence models give consistent simulation results with published experimental data by means of trend and value. Renormalization Group $k$-$\varepsilon$ model was found to give consistent simulation results with experimental data, whereas Reynolds Stress Model was failed to predict detailed features of combustion process.



## Introduction

Hydrogen is the simplest and most abundant chemical element in existence and it can be utilized as an alternative fuel [1]. Using hydrogen as fuel offers many benefits which include a reduction in the pollution levels and a drop in greenhouse gas emissions [2]. It also reduces the dependency on crude oil. When hydrogen is used in its cleanest form, the only product by combustion is water. This means exhaust gas emissions such as CO, $CO_2$, and $SO_x$ can be eliminated [1].

Considerable number of researchers investigated combustion and emission characteristics of $H_2$/air flames both numerically and experimentally. Goulier et al. [3] built an experimental setup to investigate impact of turbulence on combustion behavior of $H_2$/air mixtures. They found that turbulent flame speed is directly proportional to turbulence intensity but maximum combustion pressure is insensitive to

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**Nomenclature**

| | |
|---|---|
| $\rho$ | Density |
| $\overrightarrow{v}$ | Velocity vector |
| $p$ | Static pressure |
| $\overline{\overline{\tau}}$ and $\tau_{ij}$ | Stress tensor |
| $\rho\overrightarrow{g}$ | Gravitational body force |
| $\overrightarrow{F}$ | External body force |
| $\mu$ | Molecular viscosity |
| $I$ | Unit tensor |
| $h$ | Enthalpy of gas composition |
| $F_{hj}$ | Energy flux of the $x_j$ direction |
| $u_j$ | Velocity component |
| $\lambda_w$ | Thermal conductivity |
| $R_0$ | Universal gas constant |
| $M_i$ | Molar mass of species $i$ |
| $Y_i$ | Mass fraction of species $i$ |
| $R_i$ | Net production rate of species $i$ via chemical reactions |
| $\overrightarrow{J}_i$ | Diffusion flux of species $i$ |
| $Sc_t$ | Turbulent Schmidt number $\left(\frac{\mu_t}{\rho D_t}\right)$ |
| $\mu_t$ | Turbulent viscosity |
| $D_t$ | Turbulent diffusivity |
| $D_{i,m}$ | Mass diffusion coefficient for species $i$ |
| $D_{T,i}$ | Thermal diffusion coefficient |
| $\tau^*$ | Time scale |
| $C_\varepsilon$ | Volume fraction constant (2.1377) |
| $C_\tau$ | Time scale constant (0.4082) |
| $G_k$ | Generation of turbulence kinetic energy due to the mean velocity gradients |
| $G_b$ | Generation of turbulence kinetic energy due to the buoyancy |
| $Y_M$ | Contribution of the fluctuating dilatation in compressible turbulence to the overall dissipation rate |
| $C_{1\varepsilon}$, $C_{2\varepsilon}$ and $C_{3\varepsilon}$ | Constants |
| $\sigma_k$ and $\sigma_\varepsilon$ | Turbulent Prandtl numbers for $k$ and $\varepsilon$, respectively |
| $\alpha_k$ and $\alpha_\varepsilon$ | Inverse effective Prandtl numbers for $k$ and $\varepsilon$ (RNG model) |
| $S_k$ and $S_\varepsilon$ | User-defined source terms |
| $\mu_{eff}$ | Effective viscosity |

turbulent intensity. Thinking that laminar burning velocities are very important for design and performance of combustion systems, Ilbas et al. [4] carried out an experimental study to measure laminar flame velocities of $H_2$/air and $H_2/CH_4$/air mixtures. They concluded that an increment in $H_2$ amount in the $H_2/CH_4$ mixture increases resultant flame velocity and expends flammability limits. Jiang et al. [5] simulated hydrogen/air combustion using 3D DNS (Direct Numerical Simulation) method. Simulations were carried out in two different ways, with taking into consideration preferential diffusion and with unity Lewis number assumption. Comparisons between two different computational cases showed that preferential diffusion makes flow more turbulent. Hariharan et al. [6] performed an experimental study to understand effect of burner geometry (circular and elliptic) on performance of turbulent $H_2$/air flames. They also made some measurements to investigate flame stability characteristics and $NO_x$ emissions. They reported that because liftoff velocity is lower for elliptic burner flames, elliptic burner flames are shorter and radiate less. They also reported that for both type burners, an increment in equivalence ratio decreases NO levels. Choudhuri and Gollahalli [7] investigated characteristics of $H_2$/HC diffusion flames. It was founded that increasing hydrogen amount in fuel/oxidizer mixture increases reactivity hence combustion time and flame length reduce; an increment in hydrogen concentration rises NO and $NO_x$ emission indices but decreases CO emission index and axial soot concentration. Hwang et al. [8] investigated impact of turbulence intensity of an air stream on characteristics of hydrogen/air jet flames. Results showed that increasing turbulence intensity shortens flame length. Skottene and Rian [9] simulated $NO_x$ generation in $H_2$/air flames. For this purpose, eight laminar flames were tested with 4 different reaction mechanisms and results obtained from this numerical study were validated with experimental data in literature. They reported that generation of NO through NNH radicals is dominant NO generation mechanism for such flames. To establish dynamics of $H_2$/air flames at elevated temperatures and pressures, Kwon [10] numerically investigated laminar burning velocities of $H_2$/air flames and effect of stretch on such flames at fuel lean equivalence ratios, high pressures (5–50 atm) and high temperatures (298–1000 K). They observed that flame stretch increases laminar burning velocity up to 28%.

Increasing demand for micro scale power sources is driven by recent developments in micro devices. Compared to conventional batteries, energy intensity of these power sources is at massive levels. Micro power sources exploit from conductive and radiative heat emanating from hydrogen or hydrocarbon combustion in a micro combustor. Aside from large or mesoscale combustion applications, the subject of using hydrogen as a fuel for micro combustors is investigated by many researchers [11].

Hua et al. [12] carried out simulation studies on premixed $H_2$/air flames in a number of chambers by varying chamber dimensions and keeping aspect ratio at a constant value. They varied combustion chamber dimensions from millimeter to micron level to understand micro-combustion mechanism. They also analyzed impact of heat transfer conditions and found that the smaller the combustor size, the more effect on combustion characteristics. Li et al. [13] simulated premixed $H_2$/air combustion in micro channels. They investigated respective effects of different physical and boundary conditions on flame temperature. Numerical results showed that flame temperature is directly proportional to combustor size and at a certain inlet velocity, a flame with least temperature can be maintained. Yang et al. [14] numerically analyzed effect of reduced pressures on combustion characteristics of fuel lean hydrogen/air flames in a micro combustor with cavity and concluded that combustion efficiency follows a non-monotonic trend depending on the pressure value. When pressure decreases from 1.0 atm to 0.8 atm; combustion efficiency increases but further decrement (from 0.8 to 0.5 atm) reduces combustion efficiency. At 0.8 atm, the amount of heat released from fuel increases with rising burning velocity. But at 0.5 atm, pressure decrement has a negative effect on burning rates, reaction intensity and temperature levels. Wan