

NUMERICAL STUDY OF SYNGAS PREMIXED FLAME STRUCTURE AND EXTINCTION

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Abstract

This paper presents a numerical investigation of extinction limits (quenching and blow-off) and laminar flame speed for synthetic gas (syngas) premixed flame structure. These properties are important in premixed combustion which can be applied in gas turbines combustion chambers and burners design and modeling. Variations in syngas composition, the content of its dilution, and operating condition can have considerable impact on engine performance. Calculations are performed with using Davis et al. kinetics mechanism and a comprehensive study on effects of preheating temperature, composition, pressure, N₂, and CO₂ diluents are done for both properties. Counterflow premixed flame model is used for calculation of extinction limits. PREMIX code is used for laminar flame speed calculation and OPPDIF code for estimation of quenching and blow-off limits. Calculations show that with increasing preheating temperature, pressure, and decreasing the level of dilution with N₂ and CO₂, laminar flame speed increases and extinction limits (quenching and blow-off) become extended.

Introduction

Synthetic gas (syngas) is being recognized as a viable energy source worldwide, especially for stationary power generation. Syngas is formed through gasification processes, and can be produced from virtually any fossil fuel, including coal, biomass, organic waste, and refinery residual. Syngas fuels are typically composed primarily of H₂ and CO, and may also contain small amounts of CH₄, N₂, CO₂, H₂O, and other higher order hydrocarbons [1]. Syngas is particularly attractive for stationary power generation, since it allows for a wide flexibility in fossil fuel sources, and most of the harmful contaminants and pollutants can be removed in the post-gasification process prior to combustion. Moreover, improvements in gas turbine efficiency and reliability have made syngas a viable fuel for electric power generation using Integrated Gasification Combined Cycle (IGCC) systems [2].

Combustion and emission characteristics of premixed syngas-air mixtures have been studied widely. Natarajan et al. [3] reported measurement and computation of laminar flame speeds of H₂/CO/CO₂ mixtures over a range of fuel compositions, lean equivalence ratios, and reactant preheat temperatures. Alavandi and Agrawal [4] investigated experimentally the lean premixed combustion of CO/H₂/CH₄/air mixture, and observed that at a given flame temperature, the presence of CH₄ in a CO-H₂ mixture increases CO and NO_x emissions. J. Natarajan et al. [5] measured flame speeds for H₂/CO mixtures diluted with CO₂. Counter flow (opposed jet) geometry has been used to study H₂/O₂ diffusion flame structure and extinction limits. Most of the previous studies have dealt with systems involving undiluted or diluted hydrogen (with CO₂, or N₂) against an air flow under a variety of conditions such as

strain rates, inlet temperature and pressure. The effects of N₂ dilution for H₂/air diffusion flame were also studied. Emission characteristics of NO_x for counterflow syngas diffusion flames with airstream dilution studied by Daniel E. et al. [6]. Also a numerical and experimental study of counterflow syngas flames at different pressures conducted by S. Som et al. [7]. Jackson et al. [8] studied the effects of H₂ addition to lean premixed CH₄ flames in highly strained fields. They performed counterflow burner experiments and numerical simulations.

The purpose of this study is to extend the investigation of laminar flame speed and extinction limits for H₂/CO/Air premixed flames. Laminar flame speed for H₂/CO mixtures over wide ranges of fuel composition, equivalence ratio, CO₂ and N₂ dilutions, and reactant preheating are calculated with using model predictions based on Davis et al. mechanism [9], which is composed of 30 reactions and 14 species. Since Davis et al. mechanism does the best job in predicting the laminar flame speeds for a wide range of conditions, and also shows fairly good agreement with the measured temperature profile for a non-premixed syngas flame; it is used further in this work to study the flame structure. Moreover, this mechanism did an appropriate role in prediction of autoignition delay time among other kinetics mechanisms such as GRI 3.0 mechanism [10], San Diego mechanism [11], and Li et al. mechanism [12] in our previous study [13]. The calculated flame speeds are compared to experimental predictions. The experimental data were obtained from works of Sun et al. [14], McLean et al. [15], Bouvet et al. [16], Natarajan, et al. [5], and Hassan et al. [17].

Extinction limits which consist of quenching and blow off are also investigated for H₂/CO/Air counterflow premixed flames at a variety of conditions including the inlet temperatures, pressures, N₂ dilution, and CO₂ dilution levels. Blow-off limits, that is, extinction due to insufficient gas residence time at large stretch rates (or strain rates). The blowoff limit is obviously important in high-speed flow and in high-intensity turbulent flames containing flamelets. On the other hand, the quenching limits of premixed flame in weak flames under slow convection or at small stretch rates are also important to study. Similar to laminar flame study, Davis et al. mechanism [9] is selected for extinction limit simulations. Laminar flame speeds and counterflow flame structures have been studied using PREMIX [18] and OPPDIF [19] codes respectively, all developed by Sandia National Laboratory.

Physical and Numerical Models

Laminar Flame Speed

Laminar flame speed is used to characterize the combustion of various fuel-oxidizer combinations and in determining mixture flammability limits. Therefore, the ability to model chemical kinetics and transport processes in these flames is critical to flammability studies, interpreting flame experiments, and to understanding the combustion process itself. Computations of unstretched laminar burning velocities are performed using the PREMIX [18] code. The model solves the set of governing differential equations that describes the flame dynamics using implicit finite difference methods, as well as, combination of time-dependent and steady-state methods. The solver algorithm employed automates coarse-to-fine grid refinement as a mean to enhance the convergence properties of the steady-state approach and as a mean to provide optimal mesh placement [18]. The governing conservation equations for one dimensional flow with uniform conditions reduce to:

Continuity:

$$\dot{M} = \rho u A \quad (1)$$

Energy:

$$\dot{M} \frac{dT}{dx} - \frac{1}{c_p} \frac{d}{dx} \left(\lambda A \frac{dT}{dx} \right) + \frac{A}{c_p} \sum_{k=1}^K \dot{\omega}_k h_k W_k = 0 \quad (2)$$

Species:

$$\dot{M} \frac{dY_k}{dx} + \frac{d}{dx} (\rho A Y_k V_k) - A \dot{\omega}_k W_k = 0 \quad (k = 1, \dots, K_g) \quad (3)$$

Equation of state:

$$\rho = \frac{P\bar{W}}{RT} \quad (4)$$

For freely propagating flame, \dot{M} is an eigenvalue and must be determined as a part of the solution.

Counterflow Flame

Steady, axisymmetric, laminar flow of two counterflowing streams toward a stagnation plane is considered. Two flame types are used in the present study, a nonpremixed and a premixed configuration. They are characterized by the arrangement of the reactants among the two inflowing streams, in particular whether air is introduced into the top or into the bottom duct. The tangential components of the flow velocities at the boundaries are presumed to be equal to zero (plug-flow boundary conditions). The velocities of the fuel and oxidizer streams are chosen to conform to the global strain rate

$$a_s = \frac{2|V_O|}{L} \left(1 + \frac{|V_F| \sqrt{\rho_F}}{|V_O| \sqrt{\rho_O}} \right) \quad (5)$$

and to satisfy the momentum balance

$$\rho_O V_O^2 = \rho_F V_F^2 \quad (6)$$

here V and ρ represent the velocity and density, respectively, with the subscripts 'O' and 'F' indicating the oxidizer and fuel streams, respectively, and L is the separation distance between the two nozzles, and is taken as 1.27 cm. Using these two equations, the fuel and air stream velocities can be computed for a given strain rate. At non-premixed counterflow configuration oxidizer is air and fuel is H₂/CO and in premixed counterflow configuration fuel is CO/H₂/air and oxidizer is nitrogen.

For counterflow flame simulations, another OPPDIF code [19] is used. In the analysis of counterflow flame, the conservation equations are reduced to a boundary value problem. The one-dimensional model then predicts the species, temperature, and velocity profiles in the core flow between the nozzles (neglecting edge effects). Here, assumption of stagnation point potential flow and boundary layer are made. In this approach the strain field is characterized only by the potential flow velocity gradient. Even if most of flame experiments have not reproduced the ideal flow, realized in the analysis, comparison of strained flame experiments can be made with acceptable accuracy. The mass conservation for the steady state is the following [19]:

$$\frac{\partial(\rho u)}{\partial x} + \frac{1}{\xi^{n-2}} \frac{\partial(\rho V_\xi \xi^{n-2})}{\partial \xi} = 0 \quad (7)$$

Where u and V_ξ are the axial and the cross-flow velocity components. If V_ξ/ξ and other variables are functions of x only then:

$$G(x) = \frac{\partial V_\xi}{\partial \xi}, F(x) = \frac{\rho u}{(n-1)} \quad (8)$$

The continuity equation for axial velocity u reduces to:

$$G(x) = \frac{dF(x)}{dx} \quad (9)$$

Momentum equation with $H = \frac{1}{\xi^{n-2}} \frac{\partial P}{\partial \xi} = \text{constant}$:

:

$$H - (n-1) \frac{d}{dx} \left(\frac{FG}{\rho} \right) + \frac{nG^2}{\rho} + \frac{d}{dx} \left[\mu \frac{d}{dx} \left(\frac{G}{\rho} \right) \right] = 0 \quad (10)$$

Energy equation:

$$\rho u \frac{dT}{dx} - \frac{1}{c_p} \frac{d}{dx} \left(\lambda \frac{dT}{dx} \right) + \frac{\rho}{c_p} \sum_{k=1}^K c_{pk} Y_k V_k \frac{dT}{dx} + \frac{1}{c_p} \sum_{k=1}^K h_k \dot{\omega}_k = 0 \quad (11)$$

and species equation:

$$\rho u \frac{dY_k}{dx} + \frac{d}{dx} (\rho Y_k V_k) - \dot{\omega}_k W_k = 0 \quad (12)$$

The boundary conditions employed are the mixture composition, temperature and the inlet velocity. Symmetry conditions are applied at the stagnation or symmetry plane.

Result and Discussion

Laminar Flame Speed

Figure 1 presents numerical laminar burning velocities for 50% H₂-50% CO mixture at $P = 1$ atm, and $T = 298$ K versus several equivalence ratios for Davis et al. [9] kinetics mechanism. The results are compared with measured laminar flame speeds. The experimental data are obtained from works of Sun et al. [14], McLean et al. [15], Bouvet et al. [17], Natarajan, et al. [5], and Hassan et al. [17]. The computational model included thermal diffusion and multi component transport. The effect of thermal radiation was also considered using an optically thin radiation model.

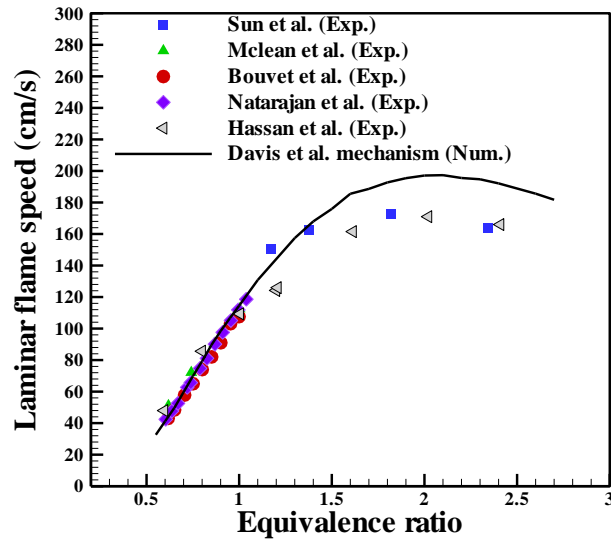


Figure 1. Comparison of measured and predicted laminar flame velocities versus equivalence ratios at $P = 1$ atm, and $T = 298$ K for 50% H_2 -50% CO mixture. Line corresponds to numerical simulation and symbols correspond to experimental data.

The Davis et al. mechanism [9] predicts the flame speeds most accurately except for the peak a value, which it over predicts slightly. Figure 2 shows a similar simulation of figure 1 for 5% H_2 -95% CO at the same conditions. Also the predictions are compared with experimental data.

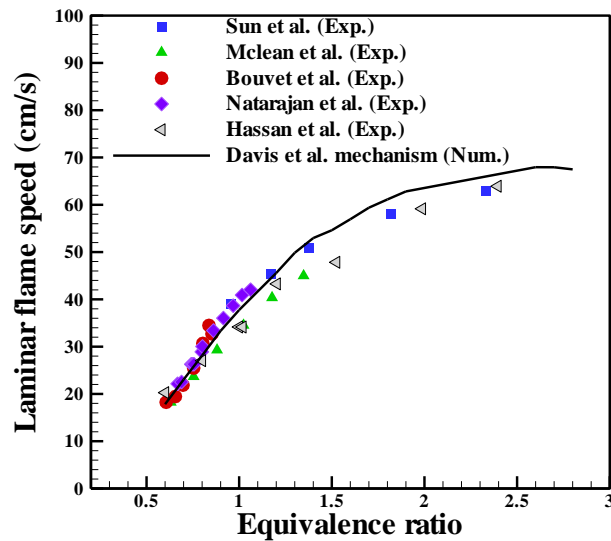


Figure 2. Comparison of measured and predicted laminar flame velocities versus equivalence ratios at $P = 1$ atm, and $T = 298$ K for 5% H_2 -95% CO mixture. Line corresponds to numerical simulation and symbols correspond to experimental data.

The agreement between simulations using Davis et al. mechanism [9] and experimental data are again excellent. As expected, the addition of hydrogen to the carbon monoxide flame raises the laminar burning velocities considerably. Since Davis et al. mechanism does the best job in predicting the laminar flame speeds for a wide range of conditions, and also shows

fairly good agreement with the measured temperature profile for a non-premixed Syngas flame; it is used further in this work to study the flame structure.

The laminar burning velocity rises significantly with an increase in reactant preheat temperatures, see Figure 3. This figure shows numerical simulation results of laminar flame speed for various equivalence ratios for Davis et al. mechanism [9]. The results are compared with Natarajan, et al. [5], experimental data.

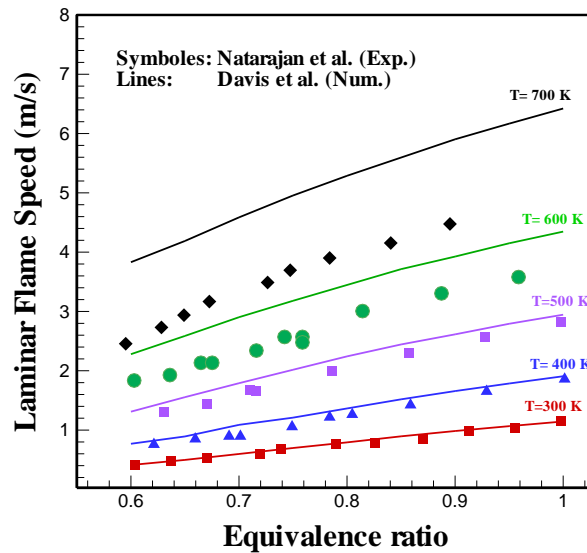


Figure 3. Comparison of measured and predicted laminar flame velocities versus equivalence ratios at $P = 1$ atm for 50% H₂-50% CO mixture. Line corresponds to numerical simulation and symbols correspond to experimental data.

Figure 4 shows the effects of N₂ addition. Addition of nitrogen into mixture results in a decrease in the laminar burning velocity, since N₂ acts as passive diluents by reducing the adiabatic flame temperature and combustion system reactivity as concentrations of reactive components (H₂, CO or CH₄) are reduced.

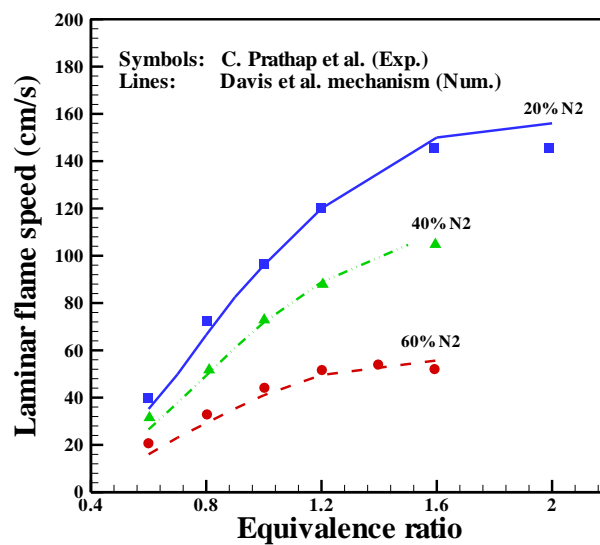


Figure 4. Comparison of measured and predicted laminar flame velocities versus equivalence ratios at $P = 1$ atm and $T = 298$ K for H₂/CO/N₂ mixtures at different N₂ dilution levels as a

function of equivalence ratio. Line corresponds to numerical simulation and symbols correspond to experimental data.

Figure 5 shows the effects of CO₂ addition on laminar flame speed. According to this figure with increasing the amount of CO₂ the laminar flame speed decreases [20]. The presence of CO₂ will impact the flame by changes in mixture specific heat and adiabatic flame temperature, chemical kinetics rates and radiation heat transfer.

The molar specific heat of CO₂ is larger than CO and H₂. Consequently, the addition of CO₂ will lower the reactant temperatures in the preheat flame region and the adiabatic flame temperature and consequently the laminar burning velocity. Since CO₂ has higher molar specific heat, its effect on the adiabatic flame temperature and burning velocity is greater in comparison to air dilution. In addition, the flammability limits and extinction strain rates of the CO₂ diluted mixtures are correspondingly narrower. CO₂ does not act as passive diluent in the fuel, it interacts kinetically. Another effect of CO₂ dilution is through higher levels of radiation as CO₂ is a more effective absorber and radiator as compared to O₂ or N₂. Therefore, CO₂ dilution can lower adiabatic flame temperature and laminar burning velocity due to radiative heat losses from the flame [20].

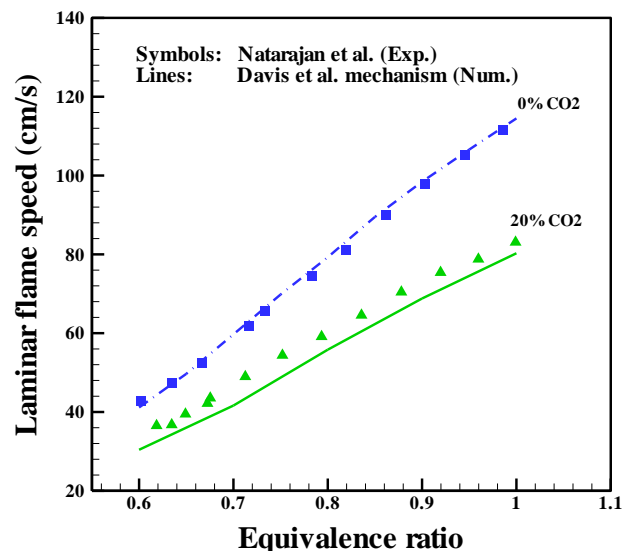


Figure 5. Comparison of measured and predicted laminar flame velocities versus equivalence ratios at $P = 1$ atm and $T = 298$ K for H₂/CO/CO₂ mixtures at different CO₂ dilution levels as a function of equivalence ratio. Line corresponds to numerical simulation and symbols correspond to experimental data.

Counterflow Non- premixed Flame

Figure 6 shows measured and predicted temperatures profiles for counterflow non-premixed Syngas/air flames established at $p = 1$ atm and $a_s = 35\text{s}^{-1}$ for 50% H₂-50% CO mixture. The numerical results include the effect of radiation for three kinetics mechanisms. Kinetics mechanisms consist of GRI 3.0 [10], San Diego mechanism [11], and Davis et al. [9]. The results of numerical simulation are compared with the experimental data which are also radiation corrected [7].

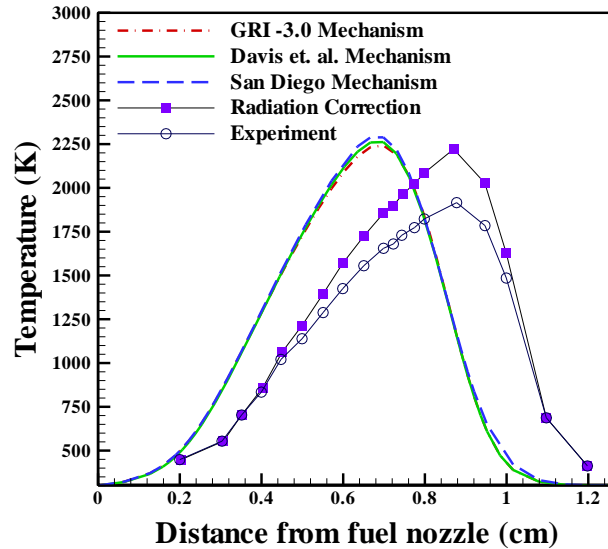


Figure 6. Temperatures versus distance from the fuel nozzle for a counterflow non-premixed syngas/air flame established at $p = 1$ atm, $T=300$ K, and $a_s= 35\text{s}^{-1}$ for 50% H_2 -50% CO mixture.

Figure 6 shows measured and predicted temperatures profiles for counterflow non-premixed Syngas/air flames established at $p = 1$ atm and $a_s= 35\text{s}^{-1}$ for 50% H_2 -50% CO mixture. The peak values predicted by GRI 3.0, San Diego Mechanism, and Davis et al. mechanisms shows that these mechanisms predict the temperature profile fairly accurately under atmospheric conditions ; however, the peaks are shifted. This is due to the strong suction employed to drain out the excess fuel [7].

Counterflow Premixed Flame

The effect of inlet temperature of premixed opposing jets flows on the extinction limits is shown in figure 7, where the maximum flame temperatures are plotted against strain rates for 50% H_2 -50% CO /Air flames at 1 atm, equivalence of 1, and different inlet temperatures. Results show, at high strain rates, the maximum flame temperatures increase and the blow-off limits are extended to higher strain rates when the inlet temperatures are increased. At higher temperatures the reaction rates increase leading to the fuel consumption acceleration, the heat release rate increase and acceleration of overall combustion process. In addition, a flame can be sustained in the higher strain fields as the main chain propagation reactions can be initiated faster due to higher reaction rates, where it would not have sufficient time at lower temperatures.

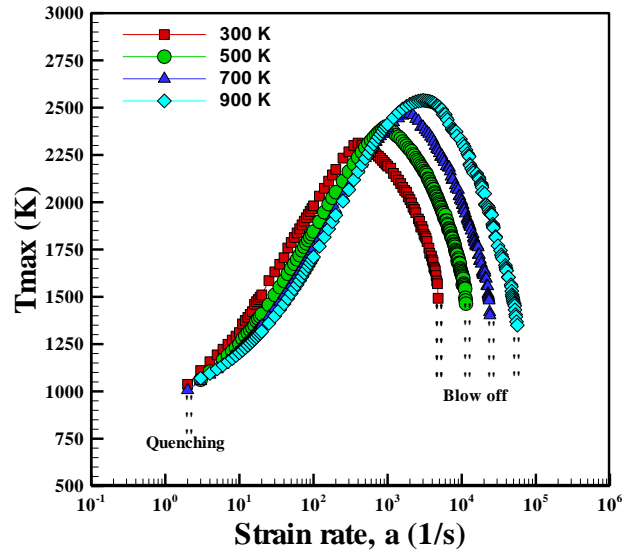


Figure 7. Maximum temperatures versus strain rate at different temperatures for a premixed counterflow 50%H₂-50%CO /Air flame established at p=1 atm, and equivalence of 1.

The effect of ambient pressure on the extinction limits is shown in figure 8, where the maximum flame temperatures are plotted against strain rates for 50%H₂-50%CO /Air flames at 300 K with equivalence ratio of 1 and different ambient pressure levels. Results indicate blow-off limit is extended when the ambient pressure is higher. This is expected since the molar concentrations of reactive species are larger at higher pressure, so the overall reaction rate is increased.

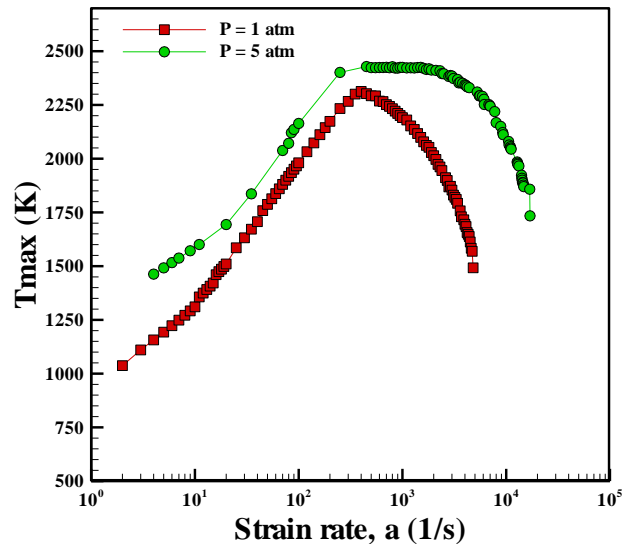


Figure 8. Maximum temperatures versus strain rate at different pressures for a premixed counterflow 50%H₂-50%CO /Air flame established at p=1 atm, and equivalence of 1.

Figure 9 shows the effects of CO₂ addition on the premixed counterflow 50%H₂-50%CO /Air flame. The effects of CO₂ addition can be considered as dilute effect, chemical effect, and radiation effect. First, CO₂ behaves simply a diluent. The addition of CO₂ reduces the concentrations of the reactants relatively, so the overall reaction rate decreases. Second, CO₂ is not totally chemically inert. It has been recognized, at high temperature, the conversion of

CO₂ to CO may appear, and the CO-related reactions cannot be neglected. Third, CO₂ is a strong radiation-participating gas. Radiation is one of the important heat transfer modes involved in flames, especially at low stretch rates or low-speed convective flows.

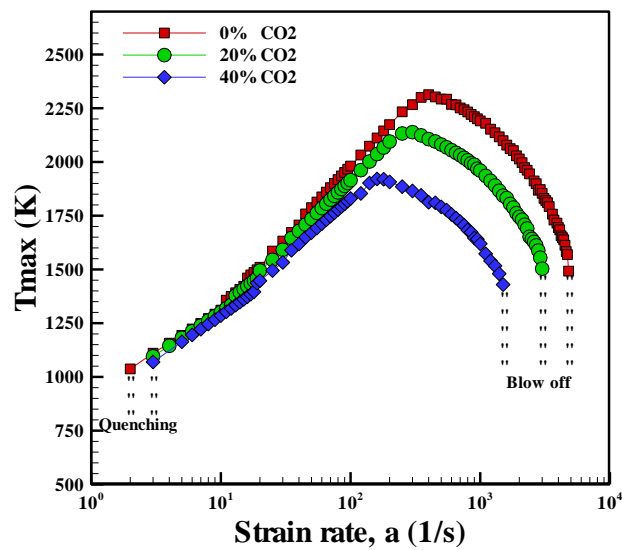


Figure 9. Maximum temperatures versus strain rate at different CO₂ dilution level for a premixed counterflow 50% H₂-50% CO / Air flame established at p=1 atm, and equivalence of 1.

Figure 10 shows the effects of N₂ addition on the premixed counterflow 50% H₂-50% CO / Air flame as dilute effect. The addition of N₂ decreases the extension of blow-off and quenching limits. N₂ acts mainly as a passive diluent, resulting in a decrease of the adiabatic temperature drop and promotion of HO₂ production and consumption reactions. N₂ also acts as a third body in the recombination reaction.

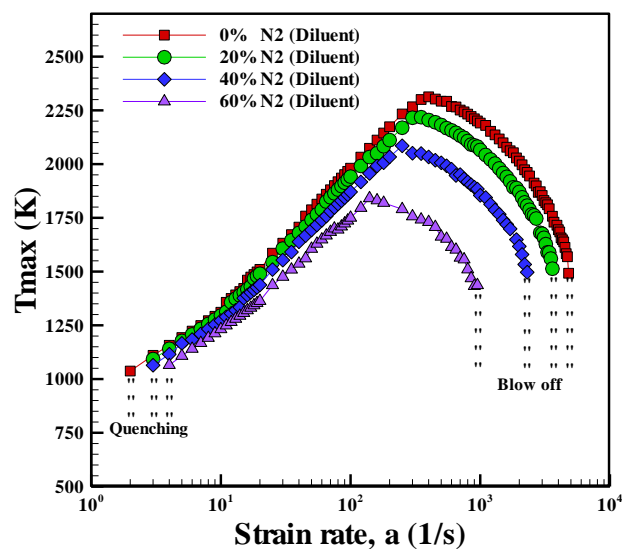


Figure 10. Maximum temperatures versus strain rate at different N₂ dilution level for a premixed counterflow 50% H₂-50% CO / Air flame established at p=1 atm, and equivalence of 1.

Conclusion

One-dimensional counterflow premixed flame and Laminar flame speed of Syngas/Air have been numerically solved with comprehensive study on effects of preheating temperature, composition, pressure, N₂, and CO₂ diluents. Calculations show that with decreasing the H₂ content, laminar flame speed decreases. Also, with increasing preheating temperature, pressure, and decreasing the level of diluents such as N₂ and CO₂, laminar flame speed decreases and quenching and blow-off limits become extended.

Results shows that the Davis et al. mechanism predicts the flame speeds most accurately except for the peak a value, which it over predicts slightly. However, it is the best kinetics model for counterflow premixed flame calculations. The addition of hydrogen to the carbon monoxide flame raises the laminar flame speed considerably. The laminar flame speed rises significantly with an increase in reactant preheat temperatures. Addition of nitrogen in to mixture results in a decrease in the laminar flame speed, since N₂ acts as passive diluents by reducing the adiabatic flame temperature and combustion system reactivity as concentrations of reactive components are reduced. With increasing the amount of CO₂ the laminar flame speed decreases the presence of CO₂ impacts the flame by changes in mixture specific heat and adiabatic flame temperature, chemical kinetics rates and radiation heat transfer. For extinction limits calculations, at high strain rates, the maximum flame temperatures increase and the blow-off limits are extended to higher strain rates when the inlet temperatures are increased.

Results indicate blow-off limit is extended when the ambient pressure is higher. This is expected since the molar concentrations of reactive species are larger at higher pressure, so the overall reaction rate is increased. The effects of CO₂ addition can be considered as dilute effect, chemical effect, and radiation effect. N₂ acts mainly as a passive diluent and its addition decreases the extension of blow-off and quenching limits.

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