

Laminar Burning Velocity and Adiabatic Flame Temperature of Biogas/Air Mixture at various CO₂ Concentrations

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1 Introduction

Combustion chambers are susceptible to the appearance of combustion instabilities that depend on the mixture properties. These instabilities are responsible for irregular combustion and are therefore disagreeable because they can damage the combustion system. It is important to know the combustion properties of the fuel in order to have better combustion efficiency and to avoid these problems. One of the key properties is the laminar flame velocity (S_L), defined as the velocity with which the unburnt gases move to the flame front. This parameter contains significant information that helps to understand reactivity, diffusivity and exothermicity of fuels. It is an important parameter in internal combustion engine modeling and combustion analysis such as the stability and structure of premixed flames, blow off and extinction of the flame, and the validation of reaction mechanisms. This paper reports some numerical results of the impact of carbon dioxide on laminar burning velocity and flame temperature of methane (CH₄)-carbon dioxide (CO₂)-air combustion. Mixtures of methane and CO₂, known as biogas, are considered as a viable alternative to replace a part of the conventional fuels. Laminar burning velocities have been numerically calculated by one-dimensional steady code using several chemical kinetic mechanisms. The laminar burning velocity and the adiabatic temperature of CH₄-CO₂/Air combustion were calculated with CO₂ concentration ranging from 0 to 50 percent in the mixture. The equivalence ratio was varied from 0.4 to 1.4, the initial pressure was set at 1 bar, and the temperature was set to 300 K. Numerical results were compared with several experimental results from the literature (Nonaka et al. [1], Zahedi et al. [2], Khan et al. [3], Bai et al. [4], Hinton and stone [5]) that investigate the effect of CO₂ increasing in biogas on the laminar burning velocity.

2 Numerical method

Numerical simulations of 1D premixed and freely propagating flame were performed using CANTERA software with several reaction mechanisms as GRI-MECH 3.0[6], San Diego[7], Blanquart et al. [8] and Aramco1.3[9] and have been compared to the experimental results of the literature. The most appropriate mechanism in terms of suitability with the experimental results in calculations below is Blanquart et al. 2018 which contains 194 species for 1156 reactions. During the computations, the chemical kinetics and transport equations for gas phase are solved following the free-propagation flame model to obtain the

laminar burning velocity and the adiabatic temperature profile. An adaptive mesh algorithm has been improved and allows adaptive mesh refinement with a defined refine criteria composed of 3 parameters which are the ratio, slope and curve with values of 3, 0.06 and 0.12, respectively, with a defined grid on the interval [0, 0.01m] with internal points determined automatically by the solver. Calculations were carried out using initial conditions of pressure and temperature of 1 bar and 300 K, which were established to determine the profiles of laminar burning velocity and adiabatic flame temperature using various chemical kinetics mechanisms for a wide range of equivalence ratios [1-5].

3 Results and discussion

First, the current numerical calculations with different chemical kinetics mechanisms were validated for CH₄/air mixtures at 300 K and 1 bar. Then, the study proceeded to CH₄-CO₂/air mixtures in order to investigate the effect of the CO₂ rate on laminar burning velocity and adiabatic temperature. Numerical results in Figure 1 are obtained with different kinetic mechanisms: GRI-MECH 3.0 [6] ; SAN DIEGO [7] ; Blanquart et al. [8] and Aramco1.3 [9] using CANTERA software. These results are compared with various experimental results from the literature [6–11] for an equivalence ratio range of (0,6-1,4). The experimental values show a good similarity with present numerical values that range from 35 cm/s to 38 cm/s. The laminar burning velocity is maximal for equivalence ratio between 1 and 1.1 and it decreases in lean and rich sides. In general, the agreement between the present numerical results and experimental values from the literature for CH₄/air mixture is good.

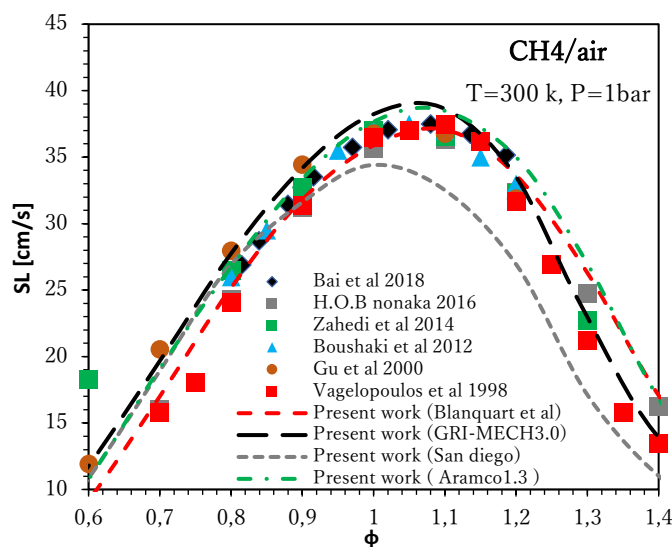


Figure 1: Laminar burning velocity (S_L) of CH₄-air with equivalence ratio at 1 bar and 300 K. Calculation results with different chemical mechanisms [6-9] compared to results from the literature [6-11].

After validating the present numerical calculations with pure CH₄-air mixtures, the present study proceeded to investigating the effect of CO₂ fraction to the mixture on the laminar burning velocity. The present numerical results of laminar burning velocities as a function of equivalence ratio for different mixtures at temperature 300 K and atmospheric pressure are plotted in Figure 2. Some experimental data of previous studies (Nonaka et al. [1], Zahedi et al. [2], Khan et al. [3], Bai et al. [4], Hinton and stone [5]) are mentioned in this figure which have been conducted in different methods. The results of numerical simulations are obtained with different kinetic mechanisms using CANTERA software. These present numerical results are compared with various experimental results from previous studies for various equivalence ratios (0,4-1,4). As CH₄-air results, the laminar burning velocity is maximal for equivalence ratio between 1 and 1.1 and it decreases in lean and rich sides for the different mixtures. On

the one hand, it is observed that numerical results performed with CANTERA with different mechanisms show a better agreement with the literature data on the lean side than the rich side. On the other hand, it is noticed that Blanquart et al.[8] mechanism predictions showed the best agreement with measurements in both rich and lean sides. The results in Figure 2 report the decrease of laminar burning velocities with CO₂ fraction. This negative effect is due to the thermal and chemical effects, The CO₂ present in the mixture acts as a diluent, so the concentration of CH₄ is reduced with the presence of CO₂ in the fuel which reduces the reaction rate and thus the laminar burning velocity.

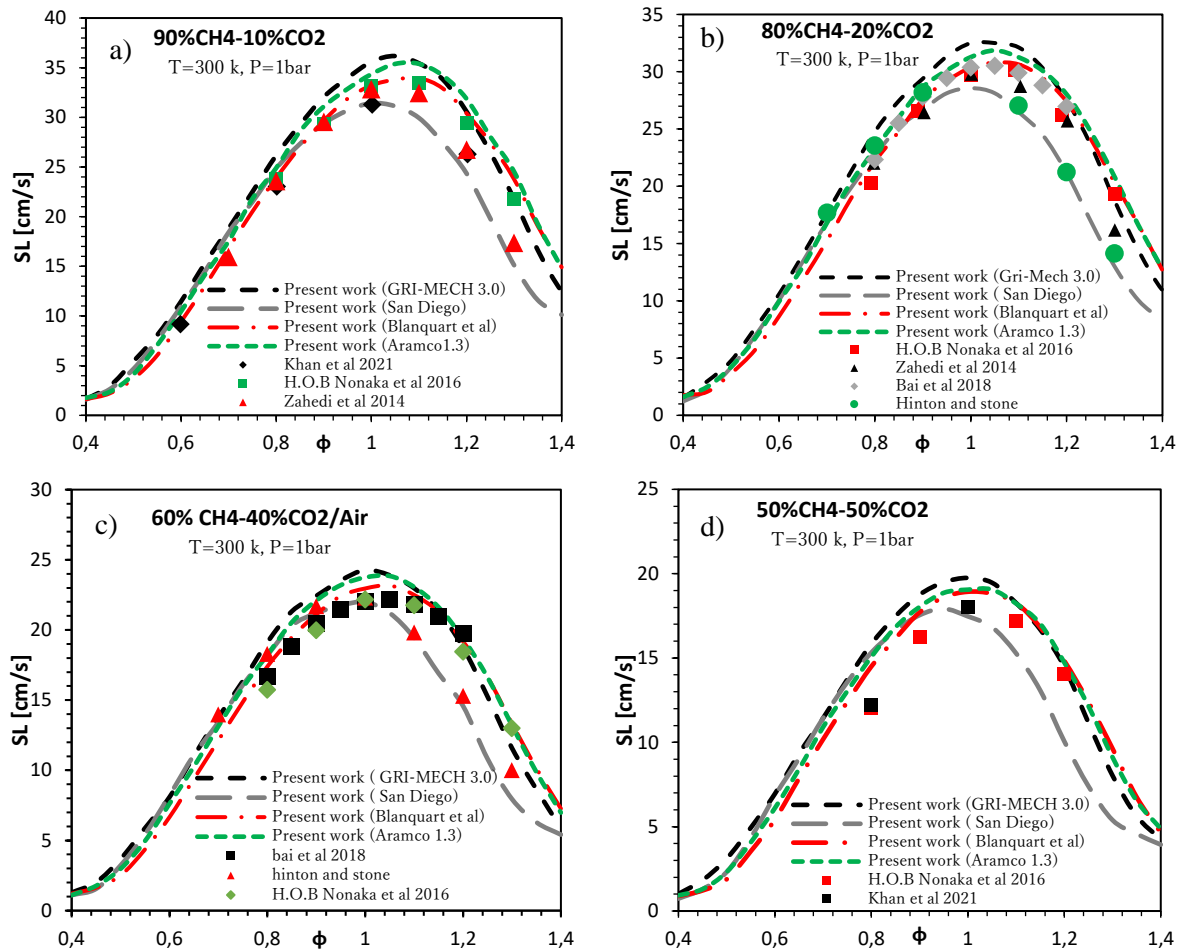


Figure 2: Laminar burning velocity (S_L) with equivalence ratio (ϕ) at 1 bar and 300 K of a) 90% CH₄-10% CO₂/air; b) 80% CH₄-20% CO₂/air; c) 60% CH₄-40% CO₂/air; d) 50% CH₄-50% CO₂/air. Comparison of numerical calculations with different chemical mechanisms [6-9] to measurements from the literature [6-8, 11, 12].

Figure 3 compares the laminar burning velocity of CH₄-CO₂/air mixture for different CO₂ concentrations versus equivalence ratio. In this figure, the numerical results are calculated by Blanquart et al. mechanism. As shown in this figure and as expected, a decrease of the laminar burning velocity is observed with an increase of the CO₂ content in the mixture. The laminar burning velocity at $\phi=1$ varies from 36 to 19 cm/s when CO₂ fraction increased to 50%. This variation reveals 47 % reduction of S_L .

Figure 4 illustrates the laminar burning velocity with CO₂ rate for three equivalence ratios 0.6, 0.8 and 1. The results show that the laminar burning velocity decreases linearly with increasing CO₂ content

from 0% to 50%. The linearity of S_L with CO_2 fraction is found for all the three equivalence ratios. With increase in percentage of CO_2 in the fuel mixture, there is a decrease in the flame velocities at all equivalence ratios, This behavior of laminar burning velocity reduction can be attributed to the high specific heat of CO_2 and to the effect of CO_2 in chemical reactions [13].

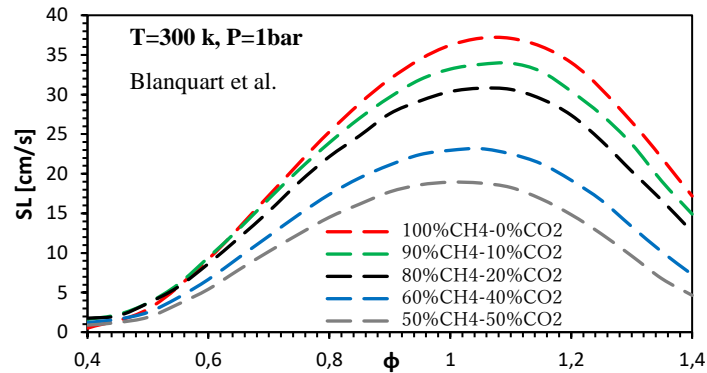


Figure 3: Evolution of calculated laminar burning velocity (S_L) using CANTERA Blanquart et al. [8] with equivalence ratio for 100% CH_4 -0% CO_2 ; 90% CH_4 -10% CO_2 /air mixtures ; 80% CH_4 -30% CO_2 /air ; 60% CH_4 -40% CO_2 /air and 50% CH_4 – 50% CO_2 /air at 1 bar and 298 K.

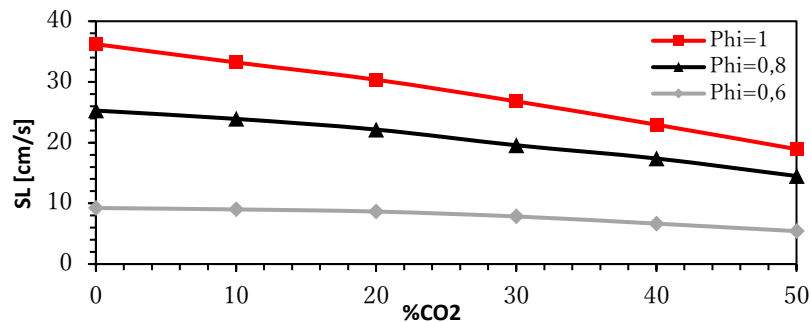


Figure 4: Laminar burning velocity (S_L) variations with carbon dioxide fraction with increasing of equivalence ratio from 0.6 to 1. Calculations with CANTERA using Blanquart et al. [8].

To clearly observe the variation of S_L with equivalence ratio at different CO_2 content at the mixture, another set of data of Kishore et al. 2008 [14] at a slightly different conditions ($P=1$ bar and $T= 307$ K) was collected and compared with our numerical results in Figure 5. The calculated results were obtained by Blanquart et al. mechanism at $T=307$ K and atmospheric pressure. Results show a good agreement with Kishore et al. results [14]. This figure clearly confirms that the kinetic mechanism of Blanquart et al. shows a good agreement with data from literature at different conditions. As mentioned earlier, the CO_2 concentration plays a negative effect on laminar burning velocity.

Figure 6 shows the evolution of the adiabatic flame temperature (T_{ad}) of CH_4 - CO_2 /air mixtures with CO_2 fraction at 300 K and 1 bar. The results show that T_{ad} decreases from 2213 K to 2056 K by increasing the volume composition of CO_2 from 10% to 50% of the mixture. In fact, CO_2 increases the thermal capacity of the mixture, which reduces the end-of-combustion temperature in addition to its diluting effect [15].

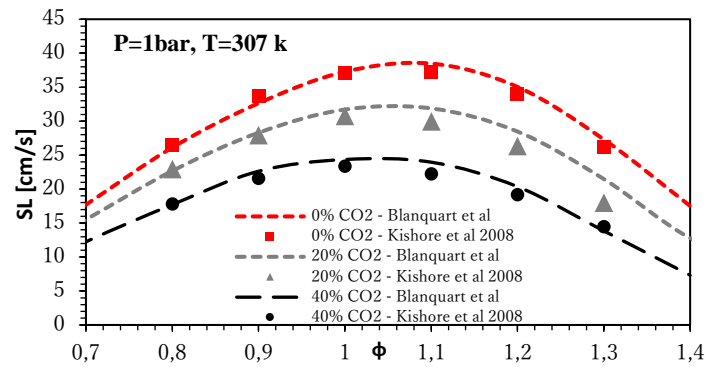


Figure 5: Laminar burning velocities with equivalence ratio for $\text{CH}_4\text{-CO}_2\text{-air}$ mixtures at $T=307\text{ K}$ and $P=1\text{ bar}$. Lines: calculations (Blanquart et al. [8]); symbols experimental data of Kishore et al. 2008[14].

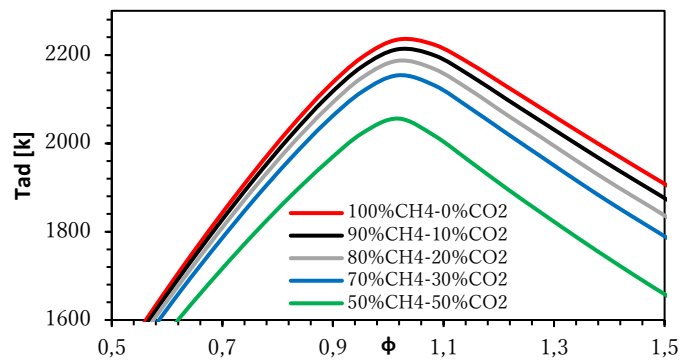


Figure 6: Adiabatic flame temperature (using Cantera GRI-MECH 3.0) with equivalence ratio for different compositions of $\text{CH}_4\text{-CO}_2$, at 1 bar and 300 K.

Pollutant emissions and laminar burning velocity of biogas combustion at different initial pressure and temperature, and with realistic conditions of an engine was also investigated, these results will be involved in the final paper.

4 Conclusions

In the present work, the laminar burning velocity and adiabatic temperature of methane and carbon dioxide mixture, the main components of biogas, was investigated numerically. Numerical calculations were performed with four detailed reaction mechanisms available in literature [6- 9]. The results were compared and validated by experimental data from the literature. From the present results, the following main conclusions can be drawn:

- Calculation results of laminar burning velocity showed more or less a good agreement with experimental data from the literature. However, Blanquart et al. mechanism values revealed the best agreement in the whole range of equivalence ratios and mixture compositions.
- The increase of CO_2 in biogas mixture decreases the laminar burning velocity and adiabatic temperature of $\text{CH}_4\text{-CO}_2\text{/air}$ combustion and this is due to CO_2 dilution and reaction effects.
- CO_2 increasing induces a little shift of the maximum burning velocity towards the lean side, and this shifting of the peak laminar burning velocity towards leaner mixtures is related to CO_2 dilution and reaction effects.

Acknowledgements

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