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Numerical Characterization of Biogas Combustion with Laminar Flame Velocity and Ignition Delay Time in Conditions Analogous to Gas Turbine Combustors

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Abstract. *Biogas is an important near-net-zero carbon fuel alternative that can reach high calorific value if subjected to upgrading and cleaning. Therefore, its composition can vary deeply depending on the level of processing performed, especially concerning carbon dioxide content. Hydrogen gas can also be present in small amounts in raw biogas and can be added to improve the fuel's calorific content. Numerical characterization of the combustion of different grades of biogas with air is performed for conditions similar to those found in gas turbine combustors with operational pressures and temperatures. Primarily laminar burning velocity and ignition delay times are calculated. Nitrogen oxides and carbon monoxide emissions are also analyzed in the range of equivalence ratios of lean premixed combustors. Combustion kinetics calculations are performed using Cantera and the reaction mechanisms for methane and air combustion used are "GRI-Mech 3.0" and "San Diego mechanism". The patterns identified for combustion characteristics and emissions layout preferred operational parameters for gas turbine combustors working with varying compositions of biogas.*

Keywords: *methane, biogas, combustion, alternative fuels, laminar flame velocity, ignition delay time*

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1. INTRODUCTION

Plenty of evidence is available about the consequences of large-scale CO_2 emissions in the atmosphere, which were shown to cause adverse and undesirable effects such as global warming. In this context, many countries are bringing more legislation into play to further restrict carbon emissions (Anderson *et al.* (2016)), which brings special interest to biofuels such as biogas. Its production is based on anaerobic fermentation of biomass from multiple origins, for example, landfills and anaerobic sewage digestors (Stanley *et al.* (2013)). Biogas, being produced from organic matter means the carbon was previously fixated by living organisms and burning it, and releasing CO_2, completes carbon the cycle without increasing the amount of CO_2 in the atmosphere. This process can even be beneficial in a way to reduce the amount of CH_4 released into the atmosphere in uncontrolled decomposition processes.

In many countries biogas already has an important economic role, for example as fuel for automobiles (Sun *et al.* (2015)), and still with a great potential for energy generation and household use in rural areas. In general, each production site produces enough fuel to meet the demand of rural communities, being an important option for distributed generation and new technologies like micro gas turbines for Distributed Energy Supply (DES) (Chen (2017)).

The digestion source for biogas production can have a great impact on its original composition. Although mostly composed of Methane and Carbon Dioxide, some amount of Hydrogen and Nitrogen can also be present (Dolejš *et al.* (2014)). Other impurities may also be present such as Hydrogen sulfide, which can lead to corrosion. Many cleaning and upgrading processes exist, which can also boost the methane content from about as low as 40% (molar) to more than 90% (Sun *et al.* (2015)). The higher fuel standard obtained by these techniques can expand the use possibilities, even improving its energy content and modifying the combustion characteristics due to the adjusted composition.

Another way to improve the fuel characteristics is by the addition of Hydrogen, which can increase flame speed and decrease ignition delay time. These properties are shown to impact processes related to gas turbine ignition in combustion chambers (Ciardiello *et al.* (2020)), flame stability (Saediamiri and Kozinski (2016)) and modify emission patterns (Fischer and Jiang (2015)).

Since the middle of the twentieth century limiting pollutant emissions like Oxides of Nitrogen, Carbon Monoxide, and unburned hydrocarbons have been a growing concern. Especially considering NOx regulations, which envision a reduction of damage to the ozone layer and smog. Since the seventies companies like General Electric are developing advanced combustion systems capable of meeting these requirements.

One possibility to control emissions is the RQL, which involves a strategy that uses a rich equivalence ratio in the primary zone, above the high NOx zone, and then, followed by a quick Quench, and subsequent lean oxidation of the ensuing carbon monoxide and unburned hydrocarbons. Therefore the technique is called RQL for Rich burn, Quench, and Lean burn (Wensheng *et al.* (2023)).

Other than the RQL strategy, at first, with NOx reduction requirements, combustors would use water injection to adequate their emissions even with penalties to its performance (Davis and Black (n.d.)). Then, with dry low NOx (DLN) and dry low emissions (DLE) systems, which operate in lean premixed configuration, some of the mechanisms of NOx formation can be avoided or reduced, such as the termic NOx (Franzelli *et al.* (2011)). These systems are called LDI (Lean Direct Injection) when only gaseous fuel is used, and LPP (Lean Premixed Prevaporized) for liquid fuels (Wensheng *et al.* (2023)).

Studying the combustion processes for different fuels and combustion strategies is essential to assess the best strategies for reducing harmful emissions and improving performance. Characterizing the fuel properties, and simulating the performance of combustion systems are the first steps towards developing cleaner combustion.

2. METHODOLOGY

2.1 Fuel Characterization

The main parameters studied in fuel characterization are the Ignition Delay Time and Laminar Flame Velocity. Although these are simulated in specific and strict conditions, these parameters are known to affect several practical aspects of burning behaviour in actual operation (Ciardiello *et al.* (2020)).

For low heat value such as lower grades of biogas stability issues can be prominent and agravated by operation at lean equivalence ratios (Huang and Yang (2009)). Having high concentration of diluents such as CO2 lead to a lower laminar flame velocity and can also cause a worse ignition performance Ciardiello *et al.* (2020).

Other cases such as the combustion of pure H2 may bring different challenges. With a relatively high laminar flame speed, flashback may be much more likely to happen (H.H.W. Funke (2019)).

Typical operational parameters for power generation gas turbines include a pressure ratio from 10.6 to 18.7 (Brooks (n.d.)). In this work, a reference operating pressure of 10 bar is chosen, which, together with an 80% isentropic efficiency of compression, gives an operational temperature of approximately 650 K. This represents the temperature of the air leaving the compressor and entering the combustion chamber.

2.2 Combustor model for Emission Calculations

The use of Chemical Reactor Networks (CRNs) for accurately modelling combustion processes is essential due to the use of detailed chemical kinetics mechanisms (Khodayari and Ommi (2020)). Using discrete reactors with different properties, particular regions of the flame can be accurately represented, connected and simulated.

The state-of-the-art of this type of analysis involves algorithms that automatically analyse computational fluid dynamics results, assign specific reactors to relevant regions and make appropriate connections to provide a complete CRN for simulations (M. Savarese (2023)).

For the scope of this work, only a premixed Lean Direct Injection (LDI) combustor is modelled, needing a, in general, less complex network in comparison to Diffusion flames (Andreini and Facchini (2004)). As shown in Figure 1, the primary combustion zone is represented as a Perfectly Stirred Reactor, followed by a plug-flow reactor. The dilution zone is considered as a quick turbulent quench, thus, modelled as a PSR. The dilution mass flow was considered for a Turbine Inlet Temperature (TIT) of 1200 K, with actual values obtained in the dilution zone ranging from 1100 to 1200 K.

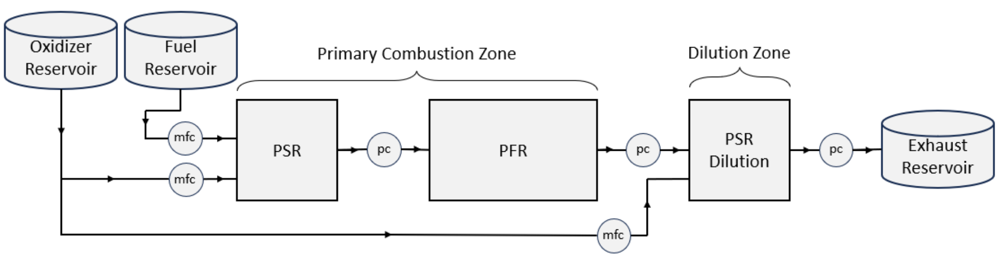


Figure 1: Chemical Reactor Network scheme for lean-premixed combustion.

2.3 Reaction Mechanisms

One of the mechanisms selected for the chemical kinetics calculations in this work is the GRI 3.0 (Smith *et al.* (n.d.)), abbreviated throughout this work as GRI. With its origins in Berkeley University, it's a detailed mechanism for methane/air combustion, with a focus on representing the formation of pollutants such as oxides of nitrogen. It consists of 53 species and 325 reactions.

Another important mechanism which was selected for analysis in this work is the "Chemical-Kinetic Mechanisms for Combustion Applications" from the University of California at San Diego (UCSD (n.d.)), referenced throughout this work as SanDiego, or simply SD. Rather than being "chemically complete", its purpose is to provide accurate and useful results for combustion simulations. It's composed of 311 reactions and 68 species with supplementary species and reactions for nitrogen chemistry.

2.4 Laminar Burning Velocity Data Validation

For validation of Laminar Burning Velocity, both numerical and experimental works were used for comparison. At ambient pressure and temperature was carried out in Figure 2 with comparisons to the results of V.K. Yadav (2019) and Benaissa *et al.* (2021). While Benaissa *et al.* (2021) presented computational results using GRI 3.0, V.K. Yadav (2019) provided experimental values using the Heat Flux Method.

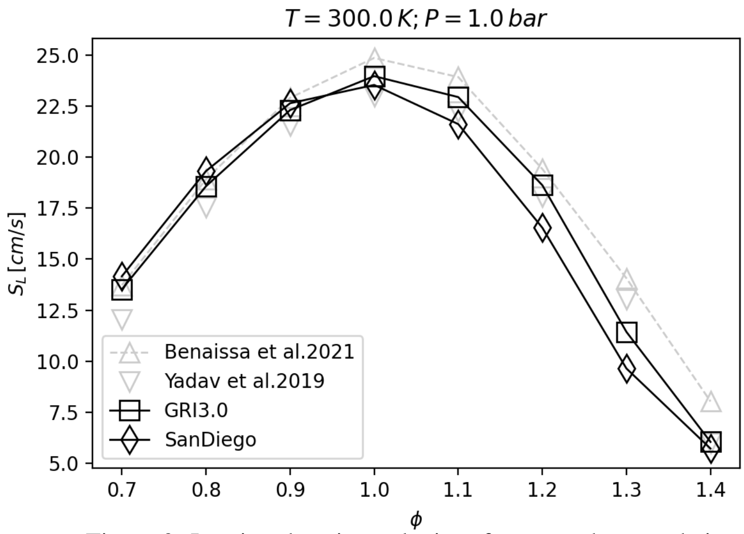


Figure 2: Laminar burning velocity of pure methane and air.

To evaluate the consistency of results at elevated pressures (5.0 bar) comparisons were carried out in Figure 3 with the results of Anggono *et al.* (2020) and M.H. Askari (2017). Both authors used the experimental technique of Spherical flame.

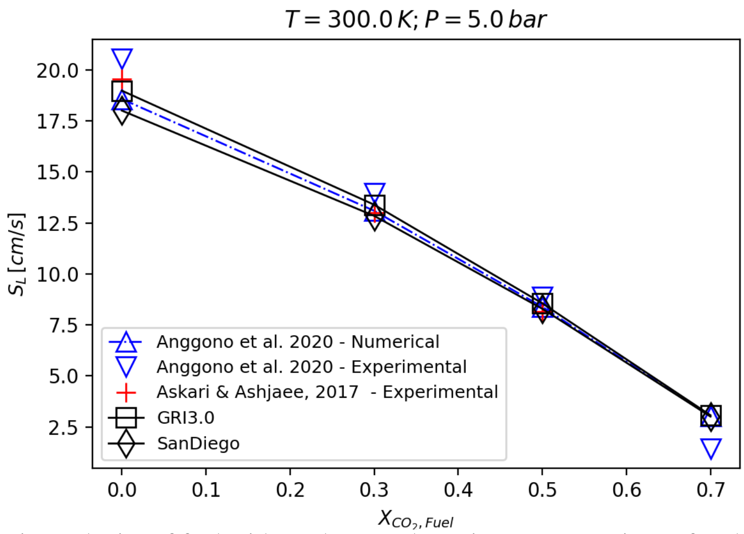


Figure 3: Laminar burning velocity of fuel with methane and varying concentrations of carbon dioxide burning with air.

With both GRI3.0 and SanDiego mechanisms there was good agreement with computational and experimental values, representing a successful validation of simulated data. In Figure 2 similar results were obtained where Benaissa *et al.* (2021) used GRI3.0 and V.K. Yadav (2019) shows experimental results with heat flux method (HFM). GRI3.0 has shown closer values to experimental data at rich equivalence ratios when compared to the results using the San Diego mechanism. Even using the same mechanism as Benaissa *et al.* (2021), a localized difference at $phi = 1.3$ is present.

Even better agreement was achieved when simulating for a pressure of 5 bar. In Figure 3 both mechanisms gave spot-on results compared to computational results with GRI3.0 from Anggono *et al.* (2020), and experimental results with spherical flames from Anggono *et al.* (2020), and M.H. Askari (2017). The best agreement was achieved with Carbon Monoxide contents from 30 to 50%.

2.5 Ignition Delay Time Data Validation

Experimental data from Heghes (2006), and Fischer and Jiang (2015)(with data from Zeng *et al.* (2014)) were chosen. Zeng *et al.* (2014) carried out shock tube experiments to determine the Ignition Delay Time of several combinations of CH4, CO2 and N2, equivalence ratios from 0.50 to 2.00 and pressures from 1 to 10 bar.

For the scope of this work values at 1.0 bar and mixture ratios of 0.50 and 1.00 where chosen for validation respectively in Figure 4 and Figure 5.

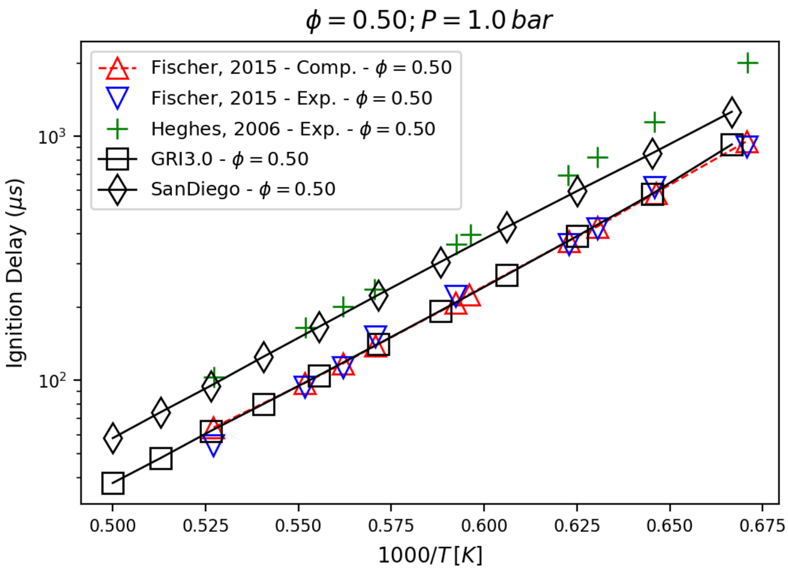


Figure 4: Ignition delay time of pure methane and air at an equivalence ratio of 0.50

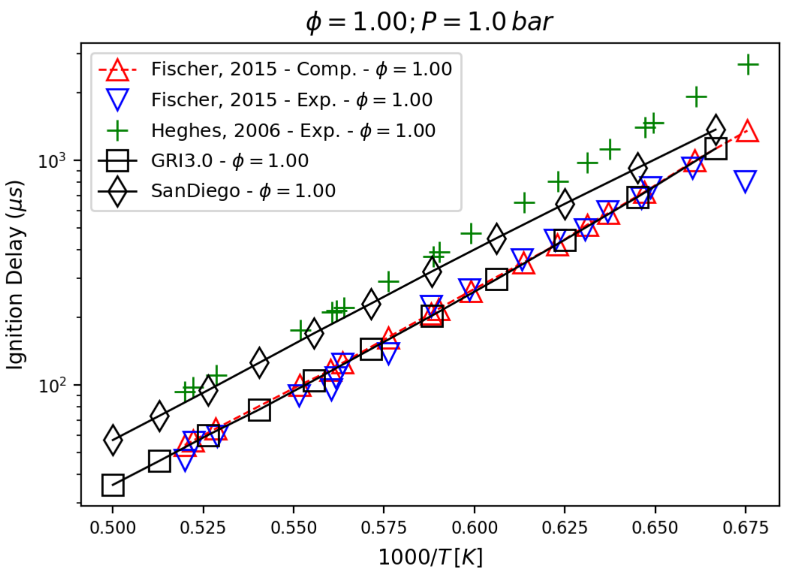


Figure 5: Ignition delay time of pure methane and air at an equivalence ratio of 1.00

3. RESULTS AND DISCUSSION

Results at gas turbine operational values show a steep difference compared to those at ambient temperature and pressure. Values of Laminar Flame Velocity, Ignition Delay Time and Emissions for LDI combustors are presented for fuel composition blends containing Methane, Carbon Dioxide and Hydrogen.

3.1 Laminar Burning Velocity

The operational parameters defined in this work have shown a great impact on the value of Laminar Burning Velocity. With much higher velocities in operational conditions, and also a slightly larger divergence between mechanisms at rich equivalence ratios. Values obtained for a composition of Methane and 20% CO2 are presented in Figure 6.

For varying concentrations of CO2 values were calculated for equivalence ratios of 0.50 and 1.00 in Figure 7. As expected, with an increase in CO2 dilution, the Laminar Flame Velocity decreased, especially at the equivalence ratio of 1.00, where the decrease was the steepest.

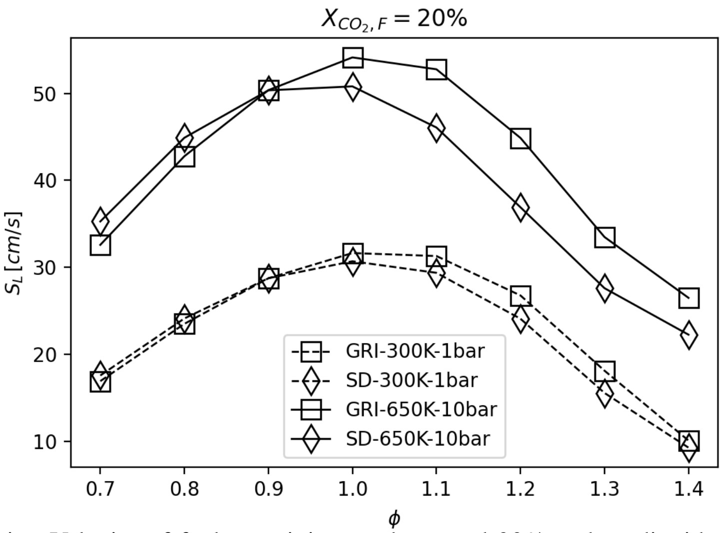
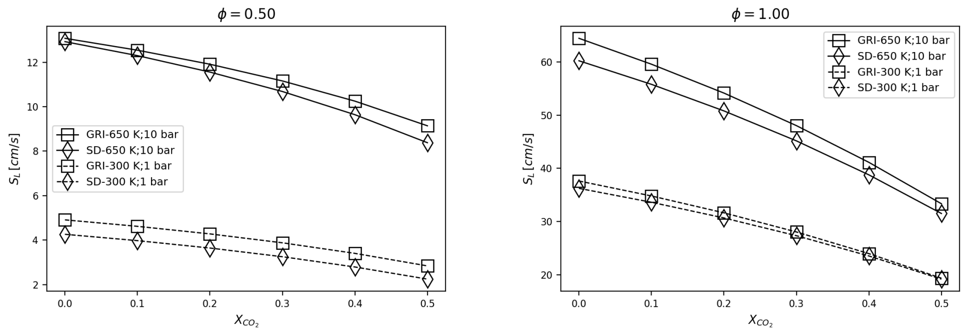


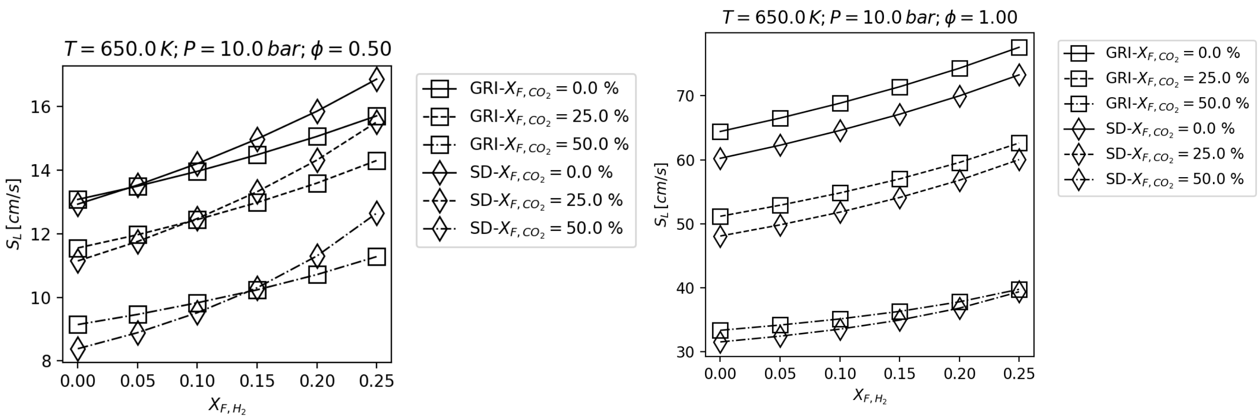
Figure 6: Laminar Burning Velocity of fuel containing methane and 20% carbon dioxide, burning with air at varying equivalence ratios.

For varying concentrations of H2 in three levels of CO2 concentration, the influence of the hydrogen on increasing the laminar flame velocity was remarkable. As shown by Figure 8, especially at lean conditions, the addition of hydrogen can compensate for higher concentrations of CO2 with respect to laminar flame velocity.



(a) (b)

Figure 7: Laminar Burning Velocity of fuel containing methane and varying concentrations of carbon dioxide, burning with air with an equivalence ratio of (a) $\phi = 0.50$ and (b) $\phi = 1.00$.

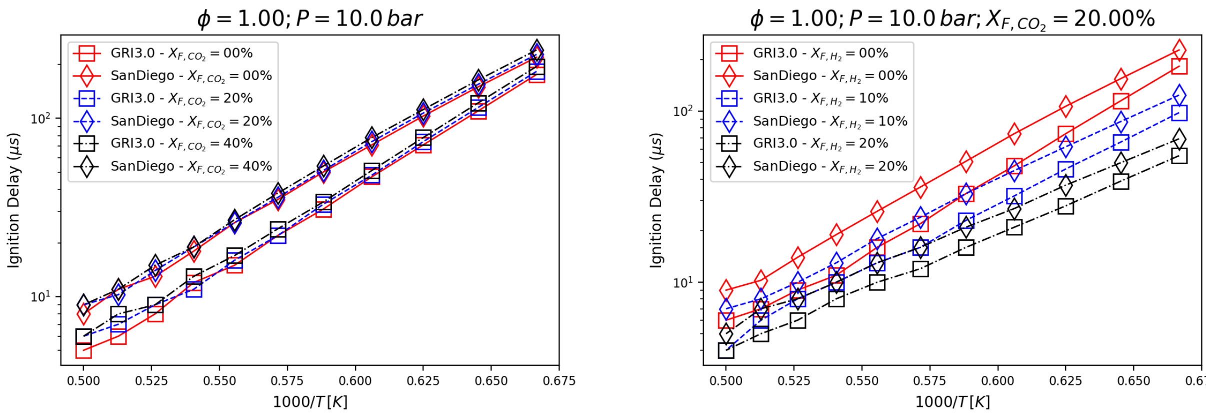


(a) (b)

Figure 8: Laminar Burning Velocity of fuel containing methane, 20% carbon dioxide, and varying concentrations of hydrogen, burning with air with an equivalence ratio of (a) $\phi = 0.50$ and (b) $\phi = 1.00$.

3.2 Ignition Delay Time

The addition of Hydrogen showed a pronounced decrease in Ignition Delay times, while the concentration of CO2 wasn't as influential. As shown by Figure 9, higher concentrations of H2 show an even larger influence at lower temperatures, indicating a possible improvement in ignition performance. The interval chosen followed these applied to fuel characterization practices since lower temperature may, in some cases, give unrealistically long IDT times which are either not representative of the ignition process, or symbolize an impracticality of spontaneous ignition at the given conditions.



(a) Varying X_{CO_2} (b) Varying X_{H_2}

Figure 9: Ignition delay time of fuel of varying compositions, (a) fuel containing methane and varying concentrations of carbon dioxide, and (b) fuel containing methane, 20% carbon dioxide, and varying concentrations of hydrogen.

3.3 Premixed Flame

Emission results for various conditions of pressure and temperature in the range of equivalence ratio useful to lean premixed combustor are presented in Figure 10. Three conditions were selected with pressures of 1, 10 and 16 bar with the equivalent temperature of the air leaving a compressor with 80 % isentropic efficiency. Carbon Monoxide emissions were neglected since all calculations led to values of less than 1 ppm in the entire interval studied.

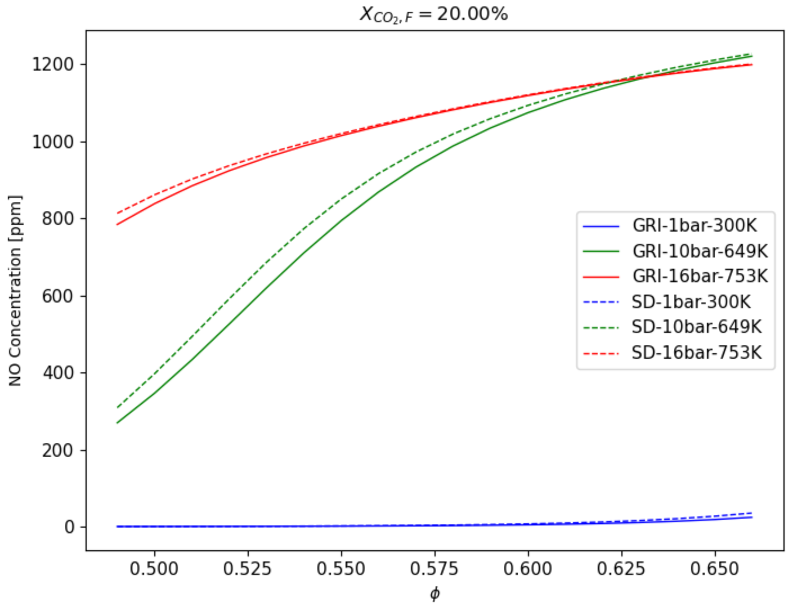


Figure 10: NO emissions for varying Equivalence ratios, pressures and temperatures.

NOx emissions were within the expected range only for the simulations in ambient conditions and increased steeply with an increase in pressure and temperature. In both high pressure cases NOx values where orders of magnitude higher than results from Lyra and Cant (2012) and Nguyen (2017). CO showed the exactly opposite trend, decreasing it's concentration in higher pressure.

Although Nguyen (2017) simulate a LPP setup, It's a similar technology to give a reference on the order of magnitude of the expected values, especially because of the technique and validation Employed. A CFD to CRN approach is performed, analyzing regions of the combustor to assign each type and properties of reactors. After that, computational results are compared to experimental data with good agreement between them, besides that, Nguyen (2017) also uses the GRI3.0 mechanism.

For varying concentrations of CO2, simulating different grades of biogas, results are shown in Figure 11. For varying quantities of Hydrogen, results are presented in Figure 12. CO2 concentration on the fuel had a great impact in NOx concentration, which may be related to lower flame temperature leading to less pronounced termic NOx formation.

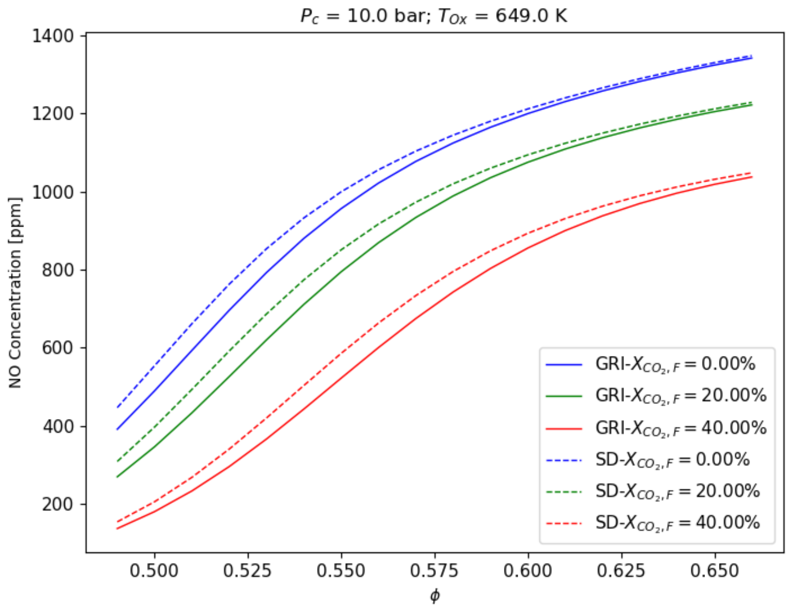


Figure 11: NO emissions for varying CO2 concentrations in the fuel.

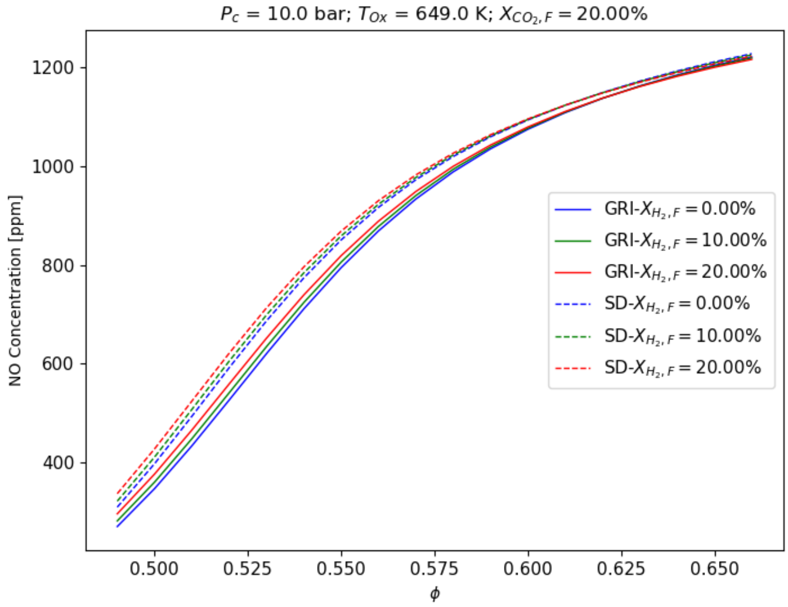


Figure 12: NO emissions for varying H2 concentrations in the fuel.

4. CONCLUSION

Both GRI3.0 and SanDiego mechanisms used throughout this work showed pertinent results towards validation and similar performance in calculations. The slight variations seem to encompass the same scale as the divergences from different experimental methods.

Considering the addition of Hydrogen to the fuel, it was confirmed that the combustion characteristics were enhanced with an increase in laminar flame velocity and a decrease in Ignition Delay Time, which may favor ignition performance and flame stability at lean premixed combustors. Although the superior flame speed may be a concern to combustor designers due to the increased possibility of flashback.

The values obtained for emissions didn't match similar simulations throughout literature, specially in relation to NOx values. In spite of providing coherent values at ambient temperature and pressure, increase in pressure and temperature following the chosen compressor modeling produced NOx concentrations orders of magnitude superior. Nevertheless, an important correlation with CO2 concentration and NOx emissions was identified where higher CO2 concentrations seem to lead to lower NOx production, probably via the reduction of flame temperature, decreasing formation via termic NOx path.

These results reinforce the sensitivity of CRN configuration for the trustworthiness of the results. Although many innovations are being created in the field of translation of CFD data to CRN building, careful analysis, testing and validation are still crucial for reliable results.

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