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Emissions and stability performance of a low-swirl burner operated on simulated biogas fuels in a boiler environment

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1 Abstract

This paper addresses the experimental and numerical modeling of NO\textsubscript{x} emissions and lean blow off (LBO) stability limits of natural gas and biogas fuels reactions stabilized with a low swirl burner (LSB). The paper presents the methodology to set up a chemical reactor network (CRN) based on experimental results and computational fluid dynamics (CFD) simulations. The CRN is a simplified representation of the fluid dynamics and energy balance of the reactive gases in the boiler environment. The CRN uses a combination of perfectly stirred reactors (PSRs) and plug flow reactors (PFRs) to couple the fluid dynamics with detailed reaction kinetics. By analyzing the CFD and CRN results, it is possible to gain insight into the relationship between internal flue gas recirculation, heat losses, geometric variables and fuel composition on the emission of NO\textsubscript{x} and the stability of the reactions. In this study, three injector configurations featuring different quarl expansion strategies were considered. Two nozzles were tested experimentally, whereas the third configuration represents an additional hypothetic design used to show the capabilities of the methodology. The numerical results are in good agreement with the experimentally observed trends and show direct relation between the emission of NO\textsubscript{x} and the lean stability limits. The quarl expansion plays a key role in the interaction of the premixed reactants and recirculated gases within the boiler environment. By varying this interaction, it is possible to attain acceptable tradeoffs between NO\textsubscript{x} emissions and burner stability. In general, the results demonstrate the ability of this design methodology to efficiently estimate burner performance and evaluate design modifications to accommodate varying fuel compositions.
Keywords: fuel flexibility; NOx emissions; lean blow off; flame stability; injector design
Emissions and stability performance of a low-swirl burner operated on simulated biogas fuels in a boiler environment

2 Abstract

This paper addresses the experimental and numerical modeling of NO\textsubscript{x} emissions and lean blow off (LBO) stability limits of natural gas and biogas fuels reactions stabilized with a low swirl burner (LSB). The paper presents the methodology to set up a chemical reactor network (CRN) based on experimental results and computational fluid dynamics (CFD) simulations. The CRN is a simplified representation of the fluid dynamics and energy balance of the reactive gases in the boiler environment. The CRN uses a combination of perfectly stirred reactors (PSRs) and plug flow reactors (PFRs) to couple the fluid dynamics with detailed reaction kinetics. By analyzing the CFD and CRN results, it is possible to gain insight into the relationship between internal flue gas recirculation, heat losses, geometric variables and fuel composition on the emission of NO\textsubscript{x} and the stability of the reactions. In this study, three injector configurations featuring different swirl expansion strategies were considered. Two nozzles were tested experimentally, whereas the third configuration represents an additional hypothetic design used to show the capabilities of the methodology. The numerical results are in good agreement with the experimentally observed trends and show direct relation between the emission of NO\textsubscript{x} and the lean stability limits. The swirl expansion plays a key role in the interaction of the premixed reactants and recirculated gases within the boiler environment. By varying this interaction, it is possible to attain acceptable tradeoffs between NO\textsubscript{x} emissions and burner stability. In general, the results demonstrate the ability of this design methodology to efficiently estimate burner performance and evaluate design modifications to accommodate varying fuel compositions.

Keywords: fuel flexibility; NO\textsubscript{x} emissions; lean blow off; flame stability; injector design

1 Introduction

Worldwide, environmental regulations to limit pollutant emissions from combustion equipment have become more stringent. Air quality legislation will become stricter in the
near future, even for combustion applications that burn clean fuels such as natural gas (NG). Improvement of combustion equipment focuses on reducing emissions, improving efficiency and lowering costs without sacrificing reliability. Advances are occurring on all three fronts, but progress is usually achieved for a single type of fuel [1]. As interest in utilizing renewably derived fuels such as biogas is increasing worldwide, development and optimization of combustion equipment to achieve minimum pollutant emission levels and maintaining stable operation as fuel composition varies is required.

Various techniques have been developed to reduce NOx emissions reduction in combustion applications. These include air or fuel staging, lean combustion [2], flameless oxidation [3], also known colorless distributed combustion (CDC), and Mild combustion [4], which shares some of the same principles of high temperature air combustion (HiTAC) [5]–[9]. Other strategies to reduce the reaction temperature include the use of internal or external flue-gas recirculation and fuel or air dilution with CO2, water steam or N2 [10]. Among the most effective in-cylinder or in chamber techniques for NOx reduction is exhaust gas recirculation (EGR). EGR acts, at part load, as an additional diluent in the unburned gas mixture [11]. EGR has been shown to reduce NOx by 80-98%. However, despite the benefits of reducing NOx emissions, the techniques mentioned can also increase specific fuel consumption, particulate emissions and unburned hydro-carbons as a consequence of the well-known NOx-bsfc and NOx-Soot trade-offs [12]. Furthermore, reducing the reaction temperature negatively affects flame stability and narrows the operating range of the combustion equipment. Mitigating the propensity of lean premixed combustors to thermos-acoustic oscillations remains a significant challenge [13]–[15]. In the case of external flue-gas recirculation (EFGR), the flue-gases added to the flame are relatively cold (~200°C) and the low temperatures of the cooled reactions become the rate-limiting factor causing reaction instabilities. Lean premixed combustion of natural gas—the most common fuel used in gas fired systems—has been successfully applied during the last few decades to achieve low NOx emissions [16]–[22]. In the case of internal flue gas recirculation (IFGR), the flue gases have a temperature similar to that of the combustion chamber [23]. In this case, the temperature is not the most important factor leading to flame instability. Instead, the aerodynamic stresses caused by the recirculation currents tend to destabilize the reaction anchoring mechanism. The boiler environment used in the present study features IFGR.
One technology that is relatively tolerant to fuel composition changes is the low swirl burner (LSB), also called low swirl injector (LSI). The LSB stabilizes a lifted flame in a velocity flow field that linearly decays along the centerline [24]–[26]. The linearly decaying flow-field matches the burning velocity of any desired fuel composition without any modification required. Hence, the burner is inherently fuel flexible.

Recent studies have studied the behavior of reactions stabilized using the LSB concept. Deng et al., characterized the flame structure, pollutant emissions and temperature distribution generated by a LSB. They examined the effect of 1) swirl number (S); three fuel compositions (C₃H₈; CH₄; and 70%CH₄+30%H₂) and thermal load. Their results suggest that both $E_{lNOx}$ and $E_{lCO}$ slightly increase as the swirl number increases from $S = 0.521$ to $S = 0.623$. In contrast, the gas composition and thermal load have more influence on the emissions of NOₓ and CO than does the swirl number [27].

Graham et al., analyzed the mechanisms for stabilization of lean premixed reactions stabilized with a low swirl burner [28]; The parameters they varied included burner geometry (nozzle diameter), swirl levels and fuel composition. Their results indicate that the dominant mechanism for stabilizing the reactions is dependent on the strength of the annular shear layer. However, their study do not relate NOₓ emissions and stability with the geometrical variables of the nozzle nor the fuel composition.

Other studies of low swirl burners have emphasized emissions performance and flame stability of the LSB [15], [27], [29]–[42]. However, a systematic examination of the coupling between this performance and the burner/boiler interface has not.

Some work associated with reactions stabilized by low swirl burners has been carried out using simulations [13], [15], [41], [43]–[48]. Simulation strategies range from time averaged methods to high fidelity direct numerical simulations. Time averaged combustion simulations usually rely on Reynolds Average Navier Stokes (RANS) models together with mixing-based, flamelet or assumed shaped probability density function (PDF) combustion models [45]. There are a number of modeling studies concerning stratified/partially premixed flames stabilized in a low swirling flow, for example using the Reynolds Averaged Navier–Stokes (RANS) equations, based on the mixture fraction and progress variable/presumed probability density function (PDF) and a RANS based flame surface density model [46], [49], [50]. In spite of the simplicity of these models, they have been successful in predicting the steady features of combustion devices, such as the
profiles of combustor exit temperatures and the steady aero-thermo-chemistry of the combustion application. However, they are unable to predict flameout and relight nor the details of pollutant formation. Since the interaction of turbulent mixing with chemical reactions occurs at the subgrid and smallest resolved scales, time resolved solutions of the large scale flow motion is necessary to assess the large scale dynamics associated with flame stabilization. As a result, LES/DNS approaches are adopted for such phenomena. The philosophy behind LES is to solve explicitly for the large (energetic) scales of the flow, directly affected by boundary conditions, whilst modeling the small (less energetic) scales of motion. DNS resolves the whole range of spatial and temporal scales of the turbulence, thus the computational cost of DNS is very high, even at low Reynolds numbers, which makes it prohibitively expensive for nearly all systems. DNS is a useful tool in fundamental research in turbulence. The use of DNS and LES allows accounting dynamically for regions of quenching/re-ignition, where unburned fuel that passed a quenched region of the flame can be consumed in the downstream high temperature region. This gives LES/DNS an advantage over RANS in that the unsteadiness of the (convectively mixing) flow is taken into account. The modeling of reactive low swirling flows using LES and DNS has been addressed elsewhere [43], [44], [46], [48], [51]–[53]. Nevertheless, less computing expensive models are also able to capture the main characteristics of the reaction structure and divergence of flow field of the low swirl reactions; Neumayer et al., [54] successfully modeled the reactions stabilized in a pressurized low swirling flow using a 2D, axisymmetric, steady state RANS coupled to the turbulent flame speed closure model (TFC) [55]. Accordingly, RANS simulations can be used to analyze the extent of EGR occurring in the combustion chamber [56] and the general features of the reactions stabilized with a LSI during steady state operation. In terms of details of stability and emissions, CFD simulations help guiding the building of the CRN, but they are not expected to predict the effect of the fuel composition on the pollutant formation (e.g., the TFC model cannot be coupled with a reaction mechanism)

In the present study, to complement the experimental work, a set of CFD simulations and corresponding chemical reactor networks (CRN) are set up to help explain the details of the emissions behavior. This methodology, sometimes referred to as a hybrid modeling approach [47], [57], has been utilized in many applications as a compromise between time efficient CFD and detailed chemical kinetics needed to establish stability behavior and pollutant formation and destruction. For CFD, the same RANS based models used by Neumayer are implemented, grounded on the success in applying these
for the LSB configuration. The corresponding CRN is a simplified representation of the fluid dynamics and energy balance of the reactive gases in the boiler environment. The CRN uses a combination of perfectly stirred reactors (PSRs) and plug flow reactors (PFRs) to couple the fluid dynamics with detailed reaction mechanism. By analyzing the experiments, CFD and CRN results is possible to gain insight into the relationships between internal flue gas recirculation, heat losses, geometric variables and fuel composition on the emission of NO\textsubscript{x} and the reactions stability. More details are provided in Section 2.3.3 below.

The objectives of the current work are: (1) to determine experimentally the relation between NO\textsubscript{x} emissions and LBO stability limits with the variation of the nozzle geometry and fuel compositions of various gaseous fuels (natural gas and biogas). (2) To apply CFD, CRNs and the experimental results to elucidate the connection between fuel composition and pollutant emissions, system heat losses, impact of internal recirculation of gases on the behavior of NO\textsubscript{x} emissions and flame stability. For the experiments, two nozzle geometries were utilized; one configuration placed the exit of the LSI 5cm inside the cylindrical nozzle, thus the premixed gas crossing the LSI enters the chamber through a sudden expansion (case I); the other geometry located the exit of the LSI 5cm in a quartl injector or conic expansion (case II).

2. Methods

The following subsections present details about the experiments and the numerical methods used to study the fluid dynamics and chemical kinetics for each injector configuration.

2.1. Low swirl burner

A need exists for fuel flexible burners that can primarily operate on one fuel but have the ability to switch to a backup fuel if the need should arise. The demand for fuel flexible injectors has driven a plethora of research and design, including the creation of the LSI and variable geometry injectors [58], [59]. Legacy injectors operated by directly injecting the fuel into the air stream and had little to no premixing of the fuel and air. These non-premixed injectors have better stability and operate more safely through fuel composition variations and flow fluctuations; however, the NO\textsubscript{x}, CO, and products of incomplete combustion (PICs) from these injectors are relatively high when compared to the emissions of lean-premixed systems.
In recent years, due in part to increasingly stringent regulations, many legacy injectors cannot meet the government-mandated requirements. Some solutions for reducing the emissions from gas-fueled applications include fuel and air staging; injectors of variable geometry and air/fuel premixing. One type of injector that can in principle, meet the fuel flexibility requirements while also achieving low pollutant emissions is the LSI. In contrast with the LSI, high swirl injectors (HSI) operate by using strong vortex breakdown in the center of the flame to provide recirculation of hot products that ignite the fresh reactants. HSI have longer residence times for the reactions in the high temperature internal recirculation zone, which inherently favors the production and release of NOx. The difference between a LSI and a HSI is: the LSI admits a portion of the premixed gases through its central channel that generates a divergent flow-field, which velocity profile decays along the center-line [24]. The linearly decaying velocity field allows the LSI to match the burning velocity of the variable composition of premixed fuels by stabilizing the reactions in a lifted flame [31]; this characteristic provides the LSI with its inherent fuel-flexibility, because the velocities along the central axis match a wide range of burning velocities without regard of the fuel composition. In one case, a LSI was set to operate on hydrogen-enriched fuels. For burning pure hydrogen the area of the central portion of the injector was decreased in order to increase the flow velocity along the centerline; with this strategy it was possible to match the high burning velocity of the hydrogen reactions [25]. Despite the change in the geometry for the most extreme case, the LSI has been demonstrated to operate on a wide range of fuels without adjustments required [60].

Regarding the configuration of the LSI, the non-swirling flow in the center of the injector naturally promotes a low level of shear stress; however the outer swirling region and the injector rim generates high shear stress regions [24]. The interaction between the injector outlet and the heat release has been observed to generate acoustically driven combustion dynamics [33]. This finding implies that vortices shed from the injector rim would enter the outer shear layer of the injector, thus causing acoustic instabilities. To limit this interaction, a LSI with quarl (conic expansion) was tested. The quarl provides a physical path for the outer shear layer region that limits flame interactions with the outer recirculation streams and blocks reflected acoustic waves.

2.2. Experimental methods

Figure 1a) shows a picture of the experimental rig. The two nozzle configurations, sudden expansion and quarl injector are presented in figures 1b) and 1c), respectively.
Figures 1d) and 1e) show two diagrams depicting the geometry of the LSI and its location with respect the sudden expansion and quarl nozzles.

The LSI installed in an optically accessible research boiler operated on NG and various biogas compositions at fixed heat input (117 kW) and variable equivalence ratio (Φ). The operating pressure was the local environment, for the University of California at Irvine it is nearly 101.3 kPa. Two nozzle configurations were tested; the first nozzle inserted the LSI 5 cm upstream of the exit plane (L_i = 5 cm) of a sudden expansion; when the quarl nozzle was used, the LSI was also placed 5 cm upstream the cone entrance. Other geometric parameters of the LSI are Injector radius (R_i = 2.6 cm); inner cylinder radius (R_c = 1.5 cm); swirler length (L_s) and channel length (L_c). Eight swirl-vanes surround the inner cylinder of the LSI at an angle (α) of 37 degrees. The central plane of the LSI has an open area of 2.6 cm², which resulted in a mass flow split ratio (m) between the inner un-swirled and outer swirled region of m ≈ 0.3. Given the above parameters and a ratio of radii $R = \frac{R_c}{R_i} = 0.56$, the swirl number (S) can be obtained using equation 1 [31]. Using that formula, the swirl number for the LSI array is $S \approx 0.46$. 

Figure 1a) Experimental boiler; b) reaction stabilized with a LSI in a sudden expansion nozzle; c) LSI in a quarl nozzle; d) diagram of the LSI in a sudden expansion; e) diagram of the LSI in a quarl nozzle. Figures 1 d) and 1 e) adapted from [31]
The boiler is mounted on an aluminum table Fig. 1a). The boiler enclosure is shaped as an octagon with sides 30.5cm wide and 91.5cm tall made entirely of stainless steel. Eight high temperature VYCOR windows provide optical access to the interior of the combustion chamber. The chamber counts with water-cooled panels used to maintain the walls at a controlled temperature. The cooling water is held below 311K with a constant flow rate of 0.56kg/s. The exhaust stack starts with the same octagonal shape as the walls, but tapers into an octagonal cone with a height of 30.5cm. The final portion of the stack is a cylinder 20.3cm diameter and 61cm height.

The air supply system can provide air up to 0.118m$^3$/s. The baseline fuel is pipeline natural gas with flows up to 0.198 m$^3$/s. Based on gas chromatography, the natural gas composition is 98% methane with remaining balance ~1% each of ethane and carbon dioxide. For the present study up to 0.00325 m$^3$/s of NG was used, corresponding to 117kW. The high heating value of the fuel is 35980.6kJ/m$^3$. The tank of liquid CO$_2$ provides a maximum flow rate of up to 0.003 m$^3$/s. A hydrogen (H$_2$) diffusion flame was used to ignite the reactions. In addition, various Omega type-K thermocouples placed flush to several locations of the walls monitored the walls and gas temperatures at different locations throughout the combustion chamber.

### 2.2.2. Exhaust gas analysis

The exhaust gas composition was measured with a Horiba gas analyzer (model PG-250). The PG-250 is capable of measuring NO$_x$, CO, O$_2$, CO$_2$, and SO$_x$ (SO$_x$ was not recorded) with a sampling frequency of 1Hz. In order to ensure accurate readings, the PG-250 span and zero calibrations were carried out each day before and after the experiments. The repeatability of the PG-250 measurements is within 0.5% for NO$_x$ and CO ranges exceeding 100 ppm and 1000 ppm. The Horiba PG-250 meets the ISO 8178 standard, which is “an international standard designed for a number of non-road engine applications. The ISO 8178 is used in many countries in the European Union, USA and Japan for emission certification and/or type approval. The uncertainty of the equipment is indicated as 0.1 ppmdv.
2.2.3. OH* chemiluminescence

The spatial distribution of OH* intensity in the flame region was recorded with an Andor I-Star ICCD camera. A narrow band-pass filter centered at 308 nm was used to isolate emission from OH*. As the LSB reaction structure is nominally axisymmetric about the centerline, the images were further post-processed with an Abel Inversion [61], [62]. The Abel inversion resolves details about the concentration of OH* in the symmetry plane (approximating a result from a planar imaging method such as Planar Laser Induced Fluorescence- PLIF). Using the technique, the volume of the flame was determined and used to guide the development of the CRN described in the following sections. Figure 2 presents the averaged OH* images obtained from the ICCD and the corresponding Abel inverted results for natural gas (top) and biogas (60% CH₄-40% CO₂) at variable φ. It is observed that the OH* intensity increases as the equivalence ratio (φ) increases and it is higher when burning pure natural gas (which is 98% methane). Adding CO₂ reduces the OH* which may also imply reduction in NOₓ emissions, since NO is produced at high local temperatures (T>1800K) by the bimolecular reaction N+OH→NO+H (Zeldovich route). Also, the inverted images show the highest concentrations of OH* in the central portion of the reaction. The numerical results show the same trends. The CFD contours confirm that most NOₓ is produced in the central portion of the reaction where the high availability of OH radicals facilitates the production of NOₓ.

Figure 2. OH* images and corresponding Abel inversions. Top row represents flame images for natural gas flames taken with OH* filter and corresponding Abel inversions about the symmetry plane. The bottom row represents a diluted biogas mixture (40%CO₂- 60%NG). The color bar legend displays the intensity of measured OH* radicals in A. U.
2.2.4. Tests matrix

A statistically based test matrix (2^3 full factorial design with repeats) was developed as shown in Table 1. The controlled variables are: equivalence ratio (ϕ), fuel composition and burner/boiler interface (sudden expansion or quarl). The measured responses are NOx and CO emissions. In addition, ϕ at LBO is determined by increasing the air flow rate until blowoff is observed. Representative NOx values are presented in table 1. To capture the lean blowoff limit, it was necessary to run leaner mixtures (not shown in the table).

<table>
<thead>
<tr>
<th>Run</th>
<th>Equivalence Ratio (ϕ)</th>
<th>NG % (Balanced CO2)</th>
<th>LSI in a sudden expansion (NOx ppmvd @ 3%O2)</th>
<th>LSI in a quarl (NOx ppmvd @ 3%O2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.95</td>
<td>60</td>
<td>10</td>
<td>22</td>
</tr>
<tr>
<td>2</td>
<td>0.93</td>
<td>60</td>
<td>8</td>
<td>19</td>
</tr>
<tr>
<td>3</td>
<td>0.95</td>
<td>60</td>
<td>9</td>
<td>21</td>
</tr>
<tr>
<td>4</td>
<td>0.87</td>
<td>60</td>
<td>7</td>
<td>14</td>
</tr>
<tr>
<td>5</td>
<td>0.92</td>
<td>60</td>
<td>8</td>
<td>16</td>
</tr>
<tr>
<td>6</td>
<td>0.95</td>
<td>60</td>
<td>9</td>
<td>21</td>
</tr>
<tr>
<td>7</td>
<td>0.86</td>
<td>80</td>
<td>12</td>
<td>27</td>
</tr>
<tr>
<td>8</td>
<td>0.95</td>
<td>80</td>
<td>21</td>
<td>44</td>
</tr>
<tr>
<td>9</td>
<td>0.86</td>
<td>80</td>
<td>12</td>
<td>28</td>
</tr>
<tr>
<td>10</td>
<td>0.8</td>
<td>80</td>
<td>7</td>
<td>19</td>
</tr>
<tr>
<td>11</td>
<td>0.8</td>
<td>80</td>
<td>8</td>
<td>20</td>
</tr>
<tr>
<td>12</td>
<td>0.95</td>
<td>80</td>
<td>20</td>
<td>46</td>
</tr>
<tr>
<td>13</td>
<td>0.77</td>
<td>100</td>
<td>6</td>
<td>22</td>
</tr>
<tr>
<td>14</td>
<td>0.95</td>
<td>100</td>
<td>30</td>
<td>54</td>
</tr>
<tr>
<td>15</td>
<td>0.95</td>
<td>100</td>
<td>29</td>
<td>56</td>
</tr>
<tr>
<td>16</td>
<td>0.77</td>
<td>100</td>
<td>6</td>
<td>21</td>
</tr>
<tr>
<td>17</td>
<td>0.95</td>
<td>100</td>
<td>31</td>
<td>61</td>
</tr>
<tr>
<td>18</td>
<td>0.77</td>
<td>100</td>
<td>7</td>
<td>19</td>
</tr>
</tbody>
</table>

2.2.5. Experimental results

Figures 3a) and b) present the NOx emissions results for each fuel plotted versus ϕ for the sudden expansion and quarl configurations (recall Fig 1), respectively. When using the sudden expansion configuration, the lowest achievable equivalence ratio (ϕ) at lean blowoff (ϕ LBO) for natural gas (pure methane~98% CH₄) was approximately ϕ~0.78. With the 80/20 (“80/20” indicates 80%CH₄ / 20%CO₂ on a volumetric basis) mixture of CH₄/CO₂ the equivalence ratio at LBO increases to ~0.80, and a 60/40 mixture increases it further to ~0.87. In contrast, when using the quarl configuration, these limits changed to ϕ~0.62 for NG; ϕ~0.65 for the 80/20 mixture; ϕ~0.72 for the 60/40 mixture and ϕ~0.8 for 50/50 mixture. It is clear that interfacing the burner to the boiler with a quarl configuration widens the stability limits of the flame. Table 2 summarizes the values of equivalence ratio.
at $\phi$ at LBO for the sudden expansion and quarl injector configurations operated on natural gas and multiple biogas mixtures.

![Graph](image)

Figure 3. Equivalence ratio ($\phi$) vs. Concentration of NO$_x$ for two injector configurations. a) Sudden expansion; b) Quarl. The heat input held constant at 117kW for all fuel compositions.

<table>
<thead>
<tr>
<th>Case</th>
<th>Fuel</th>
<th>$\phi$ at LBO</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case I - sudden expansion</td>
<td>NG~ 100% CH$_4$</td>
<td>0.8</td>
</tr>
<tr>
<td></td>
<td>Biogas 20% CO$_2$</td>
<td>0.82</td>
</tr>
<tr>
<td></td>
<td>Biogas 40% CO$_2$</td>
<td>0.88</td>
</tr>
<tr>
<td></td>
<td>Biogas 50% CO$_2$</td>
<td>Unstable</td>
</tr>
<tr>
<td>Case II - conic expansion/quarl</td>
<td>NG~ 100% CH$_4$</td>
<td>0.61</td>
</tr>
<tr>
<td></td>
<td>Biogas 20% CO$_2$</td>
<td>0.65</td>
</tr>
<tr>
<td></td>
<td>Biogas 40% CO$_2$</td>
<td>0.72</td>
</tr>
<tr>
<td></td>
<td>Biogas 50% CO$_2$</td>
<td>0.8</td>
</tr>
<tr>
<td>Case III - flush conic expansion/flush quarl</td>
<td>NG~ 100% CH$_4$</td>
<td>0.58</td>
</tr>
<tr>
<td></td>
<td>Biogas 20% CO$_2$</td>
<td>0.62</td>
</tr>
<tr>
<td></td>
<td>Biogas 40% CO$_2$</td>
<td>0.65</td>
</tr>
<tr>
<td></td>
<td>Biogas 50% CO$_2$</td>
<td>0.68</td>
</tr>
</tbody>
</table>

As expected, the concentration of NO$_x$ in the exhaust gases decreases when increasing the excess air or increasing CO$_2$ concentrations in the fuel; both of which lower
the local and overall flame temperature. For the sudden expansion configuration, near the LBO limit every fuel composition resulted in the same minimum value of NOx@LBO\sim 7ppmdv corrected to 3%O2. The CO emissions for these series of tests were within the uncertainty of the equipment (<0.1ppmdv) so were taken to be below the detection limit. During the experiments, the LBO limit was visually determined when the luminous reaction disappeared. The LBO event also resulted in a change in the sound from the reaction. Further, the concentration of NOx served as a proxy for the lean stability limit, showing minimum values close to LBO limit.

Using the injector with the quarl noticeably increased the NOx emissions for a given equivalence ratio compared to the sudden expansion configuration. However, when using the quarl, the NOx emissions were lower when operated near the extended LBO limit. When using the quarl, the minimum level of emissions for the different fuel types was found to reach a common value of approximately NOx\sim 3ppmdv at 3%O2. When using the quarl, the CO emissions for all the fuels compositions were below minimum detectable limits except for the 50% CH4 mix. In that case, CO concentrations oscillated between peaks of 15 ppmdv and zero emissions.

Figure 4 presents experimental results for the energy balance as a function of the adiabatic flame temperature. The figure compiles experimental results for biogas and natural gas. The distribution of energy flow through the combustor is almost constant regardless of the fuel type. At higher flame temperatures, it is observed an improved boiler efficiency as the heat transferred to the load increases and the sensible heat loss with the exhaust gases decreases. Approximately 50% of the heat losses correspond to 25% heat loss through the water-cooled walls and 25% through the rest of the walls including the floor.
2.3. Numerical methods:

2.3.1. Computational fluid dynamics: domain, mesh and boundary conditions

The combustion chamber geometry shown in figure 5 was simplified slightly (the octagonal cross section was represented with a cylindrical cross section) to facilitate the use of time efficient 2D CFD model for computing the fluid dynamics, heat transfer and heat release from the reactions. This strategy is consistent with the numerical results by Neumeyer [54], who successfully modeled the reactions stabilized with a LSB using RANS models. Figure 5 presents the details of the simplified geometry. A steady state, 2D axisymmetric model with swirl was used. The viscous model is the Reynolds-Averaged-Navier-Stokes (RANS), with standard wall functions. The model for radiation of species is discarded. The species model is the partially premixed model with a non-adiabatic energy treatment. The turbulent flame speed is simulated with the Zimont model. The simulations are conducted using the ANSYS Fluent, version 15. A non-structured quadrilateral mesh is used. The mesh consists of approximately 50000 cells, with a maximum aspect ratio of 2.5 and minimum orthogonal quality of 0.84. Grid sensitivity runs were carried out to ensure that the trends from the simulation were not affected by the mesh size.

Figure 4. Energy balance

Figure 5. Geometry of the virtual combustion chamber
The boundary conditions for the CFD model are set to match the energy balance of the actual system, which was calculated using a first law energy balance that uses as input the experimental measurements. This approach is useful to describe more precisely the energy flow through the chamber, which leads to a more accurate result for temperature field in the combustion chamber and therefore more precise prediction of the NOx levels.

Also, for modeling the gas injection, two mass flow inlets are used. The central portion of the nozzle is modeled with a velocity vector normal to the boundary. The annulus or swirling portion of the nozzle, including the swirl flow is modeled using a velocity vector with an axial and a tangential component. The boundary conditions presented in Table 3 were set constant for the three nozzle designs and can be used to replicate the numerical models.

<table>
<thead>
<tr>
<th>Boundary name (type)</th>
<th>Details</th>
</tr>
</thead>
<tbody>
<tr>
<td>Low swirl injector</td>
<td>Annulus or swirling portion of the nozzle</td>
</tr>
<tr>
<td>(mass flow inlet)</td>
<td>Axial component direction: 0.62</td>
</tr>
<tr>
<td></td>
<td>Tangential component direction: 0.6</td>
</tr>
<tr>
<td></td>
<td>Mass flow rate of fuel + air: 44.6g/s</td>
</tr>
<tr>
<td></td>
<td>Mass fraction through swirler vanes: 77%</td>
</tr>
<tr>
<td></td>
<td>Central portion of the nozzle</td>
</tr>
<tr>
<td></td>
<td>Flow normal to boundary</td>
</tr>
<tr>
<td></td>
<td>Mass fraction central portion: 23%</td>
</tr>
<tr>
<td></td>
<td>Conditions of the mixture</td>
</tr>
<tr>
<td></td>
<td>Equivalence ratio ((\phi)): 0.85</td>
</tr>
<tr>
<td></td>
<td>Temperature: 300K</td>
</tr>
<tr>
<td></td>
<td>Pressure: 101.3kPa</td>
</tr>
<tr>
<td></td>
<td>Fuel: 100% CH4; Oxidant: air</td>
</tr>
<tr>
<td></td>
<td>Heat input: 117kW</td>
</tr>
<tr>
<td>Water cooled wall (wall)</td>
<td>Heat output:</td>
</tr>
<tr>
<td></td>
<td>Heat transfer coefficient 300 W/m²K;</td>
</tr>
<tr>
<td></td>
<td>Free stream temperature: 300 K</td>
</tr>
<tr>
<td>Non-insulated wall (wall)</td>
<td>Heat output:</td>
</tr>
<tr>
<td></td>
<td>Heat transfer coefficient 200 W/m²K;</td>
</tr>
<tr>
<td></td>
<td>Free stream temperature: 300 K</td>
</tr>
<tr>
<td>Exhaust (outlet)</td>
<td>Pressure outlet (101.3 kPa)</td>
</tr>
</tbody>
</table>

### 2.3.2. Virtual aero-thermal field

The virtual aero-thermal field results for the three different injector configurations are compiled in Figure 6. The first row presents the three injector configurations. In the rows below each injector configuration, the temperature contours, velocity contours, and the equivalent reactor network are shown. As shown, the details of the burner interface to the boiler significantly impact the aerothermal behavior within the boiler. As a result, some insights are gained relative to the observed differences in the experimental results. For example, the wider stability limits with the internal quarl can be associated with the wider and stronger recirculation zone. However, for the present work, the primary output of the CFD results is the information needed to generate the reactor networks.
shown in the last row of Figure 6, which are used for detailed evaluation of the emissions and stability limits.

Figure 6. Virtual aero-thermal field for three nozzle designs. a) Case I: Sudden expansion; b) Case II: Conic expansion/quarl; c) Case III: Flush conic expansion or flush
The respective temperature contours for each case are presented in figures d) to f). Stream functions (right) and velocity vector fields (left) are presented in figures g), h) and i) for Case I, II and III, respectively.

2.3.3. Chemical reactor network

Chemical reactor modeling is a valuable tool in the evaluation of pollutant formation and lean blow off performance of combustion systems. The methodologies of the development vary significantly. While some researchers use simple networks made of two or three reactors [63]–[67], others use automatically generated networks that fill the fluid domain with hundreds or thousands of ideal reactors [47], [68]–[75]. In this work, the chemical reactor networks are constructed based on computational fluid dynamics (CFD) and only three or four reactors are found to be necessary to model emissions and LBO limits. For comparison, some results from automatically generated networks also are included. With a limited number of reactors, the turnaround time is significantly shorter than the automated case; a complete set of parameters including a range of air to fuel ratios can be run in minutes. For comparison, running a design point CFD and automated CRN can take days. In the present work, the experimental data were used to help in: (1) validating CFD results and (2) support the design of the network.

The concept of modeling a combustor using chemical reactors such as perfectly stirred reactors (PSR), plug flow reactors (PFR) was first introduced by S. L. Bragg [76]. A reactor network is defined to model the species formation with a detailed chemistry with a simple description of the fluid dynamics. In the present work, the GRI 3.0 reaction mechanism [77] is used for all reactor network models; GRI 3.0 is widely available and commonly used in combustion calculations. The introduction of a complex reaction mechanism in 3D turbulent combustion codes results in highly time intensive computations, which are impractical to apply in an industrial context. CFD solvers cannot be efficiently used to solve chemical equations due to the stiffness of the underlying reaction scheme and the great number of species that it contains [74]. The mathematical description of the system of equations governing a network of reactors can be found elsewhere [73]. Chemkin – Pro Release 15131 is used to solve the gas energy equation for every CRN. Matching the energy balance of the network with the energy balance of the actual system is fundamental to guarantee an accurate prediction of the emissions levels in the exhaust.
2.3.4. Zonal distribution

In order to develop the CRN, the first step is dividing the combustor volume into distinct regions or zones as guided by the CFD and experimental results. Each of the zones is characterized by the particular physical properties of the flow and the flame behavior. The two basic models used to build the network of reactors are the PSR and the PFR.

- A PSR (i.e., a continuously stirred tank reactor) presumes that mixing to the molecular scale occurs. Highly turbulent regions, premixed flows, and turbulent premixed reactions can be modeled with this type reactor. In this reactor, the chemical reaction occurs homogeneously.
- A PFR assumes that the flow moves as a “plug,” chemical reaction proceeds one-dimensionally, and longitudinal mixing in the reactor is assumed to be zero. One limitation of this model is that it can’t receive more than one stream. The composition at the entrance of the reactor has to be defined.

As shown in Figure 7, when stabilizing the reactions with the sudden expansion configuration, the first zone corresponds to the premixed flame and can be divided into two reactors. PSR1 represents the premixed region where no reaction is occurring (see temperature contours ~300K). The volume of this region is the cylinder upstream the flame zone (Vol=215 cm$^3$). In this case, PSR1 is at blow off. This means that the local conditions (temperature, pressure and the time the species spend in that region) do not trigger the initiation and chain reactions. PSR2 represents the reacting portion of the flame. The experimental OH$^*$ chemiluminescence images were used to determine the volume of the flames (Vol flame=260 cm$^3$). The volume was approximately constant for the range of equivalence ratio used with the sudden expansion nozzle. Thus, the volume of all reactors was set constant regardless of fuel composition and equivalence ratio. This is consistent with the observed reaction behavior shown in Figure 2, which indicates the overall extent of the reaction volume is not a strong function of equivalence ratio or fuel composition.

The zone downstream PSR2 is considered the immediate post flame, the temperatures in that region are the highest but also uniform. That region is still highly mixed and a zone of internal recirculation may or may not appear. The streamlines represent the trajectories of particles in a steady flow. The zones where the streamlines are circular represent recirculation zones. In the central portion of the stream the mass flow is unidirectional and better represented by a PFR. Also the contours of negative axial velocity (which are used
to find counter flow regions) show the zones where IFGR is important. Although the open center channel of the nozzle is designed to inhibit flow recirculation or vortex breakdown along the centerline [25], these features may well occur in the post flame region. The current simulations showed the formation of vortex breakdown in the centerline. Although that region is small in comparison to the outer recirculation zone. Also the contours of negative axial velocity (which are used to find counter flow regions) show the zones where IFGR is important.

![Figure 7. Contours of temperature (K) Case I (sudden expansion). PSR1 is a non-reacting premixed zone; PSR2 represents the turbulent premixed flame. PSR3 represents the recirculation zone and PFR1 the stream traveling vertically.](image)

Notice that, for the injector with quarl (case II), the main flame is insulated from the recirculation streams; therefore no recirculation loop is used in the CRN. It is assumed that the flame transfers heat to the quarl, which is cooled down by the surrounding low temperature gases (see figure 6(k)). The post flame zone is simulated with a non-adiabatic PSR (PSR3).

### 2.3.5 Reactor network variables

Each PSR in the network requires the following input variables:

- Residence time \( (R_t) \), which is the average amount of time the fluid spend in a particular system. This variable can be related to the volume \( (V) \) of the reactor, the average gas density \( (\rho) \) and the mass flow \( (\dot{m}) \) through the following expression: 
  \[
  R_t = \frac{\rho V}{\dot{m}}
  \]
- Mass flow through the reactor \( (\dot{m}) \)
- Initial temperature
- Pressure
• Heat losses

The PFRs require the following input variables:

• Length.
• Diameter. This can be a function of the distance.
• Initial temperature
• Pressure
• Heat losses

A summary of the variables used in the CRN models for the three test cases are presented in Table 4. Notice that the most important heat losses are related to the reactors close to the walls. Also the residence time indicates that the gases spend relatively long periods of time in the recirculation zones. In terms of connecting to design, species that are influenced by residence time can be impacted by altering the size and temperature of these zones.

Table 4. Boundary conditions and variables used to set up the CRNs for each fuel composition and geometry configuration

<table>
<thead>
<tr>
<th>Common parameters for all CRNs and fuel compositions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Equivalence ratio 0.5-φ&lt;1; Fuel compositions= 100%CH\textsubscript{4}; 20%CO\textsubscript{2}/80%CH\textsubscript{4}; 40%CO\textsubscript{2}/60%CH\textsubscript{4}; 50%CO\textsubscript{2}/50%CH\textsubscript{4}; Fixed heat input =117kW based on the high heating value;</td>
</tr>
<tr>
<td>PSR1: Volume=215 cm\textsuperscript{3}; PSR1 Heat losses=Adiabatic;</td>
</tr>
<tr>
<td>PSR2: Volume=260 cm\textsuperscript{3}; Inlet temperature=300 K; Pressure=101.3 kPa</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Variable parameters</th>
<th>Reactor type and number</th>
<th>PSR2</th>
<th>PSR3</th>
<th>PFR1</th>
<th>Splitter</th>
</tr>
</thead>
<tbody>
<tr>
<td>Particular parameters</td>
<td>Heat losses [kW]</td>
<td>Heat losses [kW]</td>
<td>Residence time [ms]</td>
<td>Length=90cm; Diameter=30cm; Heat losses=60kW.</td>
<td>30% to IFGR; 70% to exhaust</td>
</tr>
<tr>
<td>Case 1: Sudden Expansion</td>
<td>6</td>
<td>10</td>
<td>700</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>Case 2: Quarl</td>
<td>11</td>
<td>75</td>
<td>1000</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>Case 3: Flush quarl</td>
<td>0</td>
<td>85</td>
<td>1000</td>
<td>---</td>
<td>---</td>
</tr>
</tbody>
</table>

3. Results and analysis

Figure 8 presents experimental and numerical NO\textsubscript{x} results using (1) a manually generated CRN described above, (2) a post-CFD solution NO\textsubscript{x} model (“post-processor”) included in Fluent 15, and (3) an automatically generated CRN (“automated CRN”) (using the automated CRN feature in Fluent 15). For the three injector configurations designs, the
contours of NO$_x$ mass fraction are scaled to the same color map for ease of comparison. The first column of Figure 8 compiles the NO$_x$ results using manually generated CRNs and compares them to the experimental results. Notice that all the CFD contours represent a single operating condition (heat input: 117kW with natural gas and $\phi$=0.85) with fixed boundary conditions, except for the geometric parameter related to nozzle design. For an easy comparison, all the NO$_x$ emissions trends are framed within the same ranges of equivalence ratios and concentrations in ppmdv corrected to 3% O$_2$. The second column shows contours of NO mass fraction, as predicted by the NO$_x$ postprocessor model. This model provides the capability to simulate thermal, prompt, fuel bound, and re-burn NO$_x$ formation mechanisms. It uses rate models developed at the Department of Fuel and Energy at The University of Leeds (England) and open literature [78]. Under most circumstances, NO$_x$ variation trends can be accurately predicted with this model, however for a given operating condition the NO$_x$ quantity measured in the exhaust pipe, in general cannot be pinpointed with this model.

The third column presents NO mass fraction contours generated with Fluent's automated CRN feature. In sharp contrast with the manually generated CRN, an energy equation is not solved in the automatically generated reactor network. Instead, by default, the temperature in each reactor is calculated from the equation of state. The reactor pressure is fixed and determined as the mass-averaged pressure of the CFD cells in the reactor. This approach ensures that heat loss (or gain) in the CFD simulation is appropriately accounted for in the reactor network. For this automated network, like for the manually developed network, GRI 3.0 was used as the reaction mechanism along with its transport properties. For this network, a sensitivity analysis was carried out to determine the independence of the results to the number of reactors. 500 reactors were enough to guarantee results stability; however solving the system of differential equations for one operating condition takes around 1 hour (Processor Core™ i5-3570 CPU @ 3.40GHz/installed memory 4GB). For comparison, the manually generated network is able to provide results for the entire range of equivalence ratios and four fuels in less than 30 minutes.
Figure 8. Compiled results. Figure 8a), b) and c) CRN and experimental results against equivalence ratio for Cases I, II and III, respectively. Figures 8d) to f) NO mass fraction contours at constant boundary conditions (100% CH₄ @ φ=0.85) using CFD post-processor. Figures g) to i) NOx concentration using automated CRNs for Cases I to III (500 reactors-GRI 3.0), respectively. The color maps describe the results of each column.
3.1. Nozzle design: comparative analysis

A direct comparison of the NO contours modeled with the post-processor or the automated CRN indicates that, at a fixed equivalence ratio (ϕ=0.85), the sudden expansion configuration emits the lowest levels of NO, followed by quarl and the adiabatic quarl, respectively. Also, longer residence times of the gases in the chamber promote the formation of NOx, as the NOx formation rate is slow compared to more reactive species, such as CO or OH. The exhaust temperature also indicates that the sudden expansion configuration allows a better mixing of the hot reactants with the cooled recirculated gases, this effect reduces the stability limits as observed in Fig. 8a) when compared to fig. 8b) and 8c). Table 5 shows selected results for the numerical simulations using CFD, automated CRNs and manual CRN and experimental data.

<table>
<thead>
<tr>
<th>Variable</th>
<th>CFD results</th>
<th>Manual CRN</th>
<th>Experiments</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Residence time in the chamber [s]</td>
<td>Exhaust temperature [K]</td>
<td>NOx - CFD post-processor</td>
</tr>
<tr>
<td>Case I</td>
<td>Sudden Expansion</td>
<td>1.04</td>
<td>1276</td>
</tr>
<tr>
<td>Case II</td>
<td>Quarl</td>
<td>0.92</td>
<td>1314</td>
</tr>
<tr>
<td>Case III</td>
<td>Flush Quarl</td>
<td>1.21</td>
<td>1420</td>
</tr>
</tbody>
</table>

3.1.1. Case I - sudden expansion:

This design ensures the best interaction of the flame with the flue gas recirculation. The recirculation of combustion products into the reaction zone lowers NOx emissions by reducing the partial pressure of the oxygen in the flame zone; also the combustion reactions lose heat to the flue products by mixing-conduction, convection and direct radiation. Any strategy that reduces peak flame temperatures lowers NOx emission. In this case the outer recirculation zone is very large and the stream exchanges heat with the water-cooled walls reducing the temperature of the combustion products that return to the reaction zone. The recirculation effect is accounted with the recirculation loop (figure 6j).
When compared to cases II and III, it is clear that the recirculation stream plays a fundamental role on the total production of NO\(_x\) emissions and the stability of the flame. At \(\phi=0.93\), the NO\(_x\) emissions for case I are \(~31\) ppmvd \(\text{N}_2\) at 3% O\(_2\); at the same condition, the NO\(_x\) levels for Case II are \(~50\) ppmvd \(\text{N}_2\). Case III uses an insulated nozzle, which guarantees better resistance to blow off than a non-insulated flame. The flame can become unstable if the direct heat losses from the flame are large enough to cool down the reactions to the point where the reactions are quenched affecting the stability. At \(\phi=0.93\), the NO\(_x\) levels for case III are ~92 ppmvd @3% O\(_2\). Notice that the widest stability range of case III is also associated with higher levels of NO\(_x\) at a similar equivalence ratios for the other two cases.

These results indicate that adequate pathways for flue gas recirculation reduce the NO\(_x\) emission by 38% (case I vs. case II) when running on natural gas. However, reducing NO\(_x\) also reduces stability range. Ultra-low NO\(_x\) burners such as the low swirl burner operate at conditions that are close to the theoretical flammability limit. Close to that limit, the heat generated by the reactions is not enough to ignite the incoming mixture of fresh reactants. In low-NO\(_x\) combustor design, this limit is often bound by the onset of combustion instability in the form of LBO. As the temperature is decreased to reduce NO\(_x\), the chemical reactions slow to the point where temperature becomes the rate limiting factor and the onset of LBO is triggered. In addition to the cooling effect of the recirculation stream, it also destabilizes the flame, as the recirculation flows stress and deform outer shear layer of the flame. It is remarkable that a single CRN, with variable mass flow input (to account for equivalence ratio and the CO\(_2\) in the fuel), was able to accurately model the effect of the fuel composition for Case I.

With the sudden expansion, the flame does not attach to the nozzle port; furthermore, the exit diameter of the nozzle (rim) is the only surface area available to generate stagnation points. With this design, the LBO for NG, biogas 20% CO\(_2\) and biogas 40% CO\(_2\) happens at \(\phi_{\text{LBO}}=0.8\), \(\phi_{\text{LBO}}=0.82\) and \(\phi_{\text{LBO}}=0.88\), respectively. The sudden expansion nozzle was unable to stabilize biogas flames with 50% CO\(_2\) composition. At \(\phi_{\text{LBO}}\) the CRN predicts NO\(_x\) around 5ppmdv @ 3%O\(_2\) regardless of fuel type. For this configuration an increase of the fraction of gases recirculated through the IFGR loop shifts the NO\(_x\) emissions trends downwards, reducing the stability limits. Both NO\(_x\) postprocessor and automated CRN also indicate the sudden expansion emits the lowest NO\(_x\) emissions at a given equivalence ratio. For natural gas at \(\phi=0.85\), the postprocessor predicts 8
ppmdv and the automated CRN 38 ppmdv, the manual CRN produces the best fit for the experimental results with 15 ppmdv, all concentrations corrected @ 3% O₂.

3.1.2. Case II - conic expansion/quarl:

The quarl is a physical guide for the outer shear layer region; it stops outer recirculation, outer shear layer interactions, and blocks reflected acoustic waves. It also provides a large surface area where the flame can attach. During the experiments there was no visual access to the reactions enclosed in the quarl, however the CFD results show that for case II and III the flame is not lifted and in sharp disparity with case I, the reactions are located near the internal walls of the quarl (see figures 7e, f). Temperature contours show the regions in the chamber where the reactions are located. Those profiles confirm the proximity of the reactions to the quarl nozzle. The non-flush injector with quarl insulates the flame from mixing effects with the surroundings, but not from thermal effects. The flame is not adiabatic and transfers heat to the quarl, the former is cooled down with the recirculated gases in the chamber. The quarl widens the stability range for all fuels; it even extends the stability range to allow the burning a very low calorific value biogas with a composition of 50% CH₄-50%CO₂. The CRN for case II loses heat from the flame reactor (PSR2), but it is not affected by recirculation patterns. Insulating the flame from recirculation enhances the stability, but also the NOₓ emissions. With this design, the LBO for NG, biogas 20% CO₂, biogas 40% CO₂ and biogas 50%CO₂, happens at $\phi_{\text{LBO}} = 0.61$, $\phi_{\text{LBO}} = 0.65$, $\phi_{\text{LBO}} = 0.72$, and $\phi_{\text{LBO}} = 0.8$, respectively. Again, at $\phi_{\text{LBO}}$ the CRN predicts a NOₓ concentration ~5 ppmdv @ 3%O₂ regardless of fuel type. For biogas 50% CO₂ changing the fuel composition didn't grant the significant NOₓ reduction observed experimentally. Increasing heat losses from the flame reactor shifts the NOₓ emissions downwards; in general terms an adiabatic flame will emit the highest NOₓ levels.

3.1.3. Case III- Injector in a flush quarl:

Similarly to case II, the quarl insulates the flame from mixing effects, but this time it is assumed the reactions take place in an adiabatic control volume. The CRN for this case assume zero heat losses from PSR2. For this case all the heat losses are recharged to the PSR3 (post flame). Insulating the flame from heat losses ensures better resistance to LBO, however an adiabatic nozzle might lead to other instabilities such as Flashback. The CFD results indicate that at a fixed equivalence ratio, case III emits the highest NO concentration, followed by case II and case I with the lowest NOₓ levels. Similarly the stability ranges are enhanced. Using the CRN the estimated LBO limits for NG, biogas
20% CO$_2$, biogas 40% CO$_2$ and biogas 50%CO$_2$, happens at $\phi_{LBO} = 0.58$, $\phi_{LBO} = 0.62$, $\phi_{LBO} = 0.65$, and $\phi_{LBO} = 0.68$, respectively. Also the recirculation pattern for case III is very different to the previous cases. While cases I and II presented a small vortex breakdown in the post flame zone, case III indicates that with the flush quarl this vortex zone is enhanced. Conversely the recirculation zone in contact with the walls (clockwise rotation) is compressed to the corners. The vortex breakdown rotates counter clockwise.

Finally, key results for fuel composition effects on emissions of NO$_x$ are as follows: The concentration of NO$_x$ decreases with the addition of CO$_2$ to the fuel, with the highest levels of diluent producing the lowest NO$_x$ and highest level of CO$. The volumetric content of CO$_2$ in the fuel is one of the reasons for a diluted emissions measurement. In addition, the lower biogas flame temperatures, when compared to natural gas, reduce NO$_x$ emissions. The lower flame temperatures are a consequence of the dilution with CO$_2$, acting as a heat sink. Also the dilution of the reactions with CO$_2$ hinders the formation of radicals such as OH, and O and H atoms. A similar concept applies for IFGR, as CO$_2$, N$_2$, H$_2$O and O$_2$ recirculate into the reaction zone reducing the reaction temperature and causing NO$_x$ emissions to drop. The stability range is also affected by the addition of CO$_2$; with more CO$_2$ in the fuel the stability range becomes narrower and the LBO happens at higher equivalence ratios, compared to undiluted fuel.

4. Conclusions

- Three injector/boiler interface configurations were analyzed using CFD and CRNs, and compared to experimental results. The results indicate an unavoidable trade between NO$_x$ and stability range. Any attempt to reduce NO$_x$ emission also reduced the stability range. At a fixed equivalence ratio, the nozzle design that displayed the lowest NO$_x$ levels had the narrowest stability range. The sudden expansion configuration results in the lowest NO$_x$ levels at higher equivalence ratios since the lifted flame constantly interact with the recirculated gases. However, the stability range in relatively narrow: for natural gas the lean off limit was $\phi_{LBO} = 0.8$. Conversely, a non-adiabatic quarl or conic expansion (Case II) insulates the flame from mixing the surrounding streams, but does not shield it from thermal effects. The injector with quarl extends the LBO stability limit for NG up to $\phi_{LBO} = 0.61$. An adiabatic reaction enclosed in a quarl (case III) insulates the flame from thermal and mixing effects. For case III, the stability limit for natural gas was
\( \phi_{\text{LBO}} = 0.58 \). For cases I, II, and III fueled with NG at \( \phi = 0.93 \), reference levels for emission were 31, 50, and 92 ppmdv @ 3% \( \text{O}_2 \), respectively.

- Generally, the results illustrate the importance of considering the burner/boiler interface and overall interaction that results. Developing a low emissions burner or fuel flexible burner in absence of consideration for the full boiler geometry can result in misleading results.

- An optimized CRN model, including the effect of the flue gas recirculation, heat losses and geometric variables, is able to predict the measured changes in the emissions and lean blow off limits when changing the fuel composition (biogases up to 50% \( \text{CO}_2 \) and NG). Once the CRN is tuned with experimental results, it can be used to analyze the effect of other variable parameters on the emissions and stability limits.

- Overall, the results show that the CRN methodology can be used as a valuable tool for the design of combustion systems. The CRN is able to correlate the geometry of a system with the variables that govern the formation of pollutants (heat transfer, residence time, temperature, mixing strategy, IFGR). Therefore, it can be used as a design tool to minimizing emissions and control stability issues even as fuel composition varies.

5. Acknowledgments

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6. References


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G. P. Smith *et al.*, “GRI-MECH 3.0,” [http://www.me.berkeley.edu/gri_mech/](http://www.me.berkeley.edu/gri_mech/).

Highlights

The fuel flexibility capability of a low swirl injector is assessed in detail

The experimental boiler environment used features internal EGR

The low swirl injector self-adjusts to stabilize a wide range of fuels

A validated computational methodology is used to predict emissions and stability

The method’s utility for estimating burner performance and design impacts is shown