Effect of Variable Fuel Composition on Emissions and Lean Blowoff Stability Performance
Analysis of Nine Industrial Combustion Applications

Appendix D - Burner Configuration #4: Oxy-Fuel Burner
Burner Configuration # 4: Oxy-Fuel Burner

Emissions and Stability Performance

CEC Agreement No. 500-13-004

Prepared by:
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<td>46</td>
</tr>
</tbody>
</table>
Burner Configuration # 4: The Oxy-Fuel Burner

Executive summary

A summary of the emissions and stability results for Burner Configuration #4, the Oxy-Fuel Burner, is presented in Table 1. The table is coded with colors and trend indicators to provide a simple overview of how fuel composition impacts the performance of Burner Configuration #4.

Table 1: Summary of emissions and stability

<table>
<thead>
<tr>
<th>Fuel type</th>
<th>NOx</th>
<th>CO</th>
<th>Stability</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Hydrogen enriched natural gas (CH$_4$+H$_2$)</td>
<td>↑@↑H$_2$</td>
<td>↓@↑CO$_2$</td>
<td>-</td>
</tr>
<tr>
<td>2 Biogas (CH$_4$+CO$_2$)</td>
<td>↓@↑H$_2$</td>
<td>↓@↑CO$_2$</td>
<td>↓@↑CO$_2$</td>
</tr>
<tr>
<td>3 Mixtures with heavier hydrocarbons (C$_2$H$_6$, C$_3$H$_8$)</td>
<td>↑@↑C$_2$H$_6$, C$_3$H$_8$.</td>
<td>↑@↑C$_2$H$_6$, C$_3$H$_8$.</td>
<td>-</td>
</tr>
</tbody>
</table>

1 Cells highlighted with red represent negative impacts on emissions or stability. Conversely, cells highlighted with green represent positive effects. Those cells only containing a dash pretend to express that no blow off instabilities have been detected.

2 Fuel Type 1: Hydrogen Containing Fuels.
Fuel Type 2: Diluted Fuels.
Fuel Type 3: Fuels with Higher Hydrocarbons.

The example below illustrates how the Table 1 can be read:

<table>
<thead>
<tr>
<th>Emissions</th>
<th>Hydrogen enriched natural gas (CH$_4$+H$_2$)</th>
<th>Reading</th>
</tr>
</thead>
<tbody>
<tr>
<td>NOx</td>
<td>↑@↑H$_2$</td>
<td>NOx increases (↑) when adding (↑) H$_2$</td>
</tr>
<tr>
<td>CO</td>
<td>↓@↑H$_2$</td>
<td>CO decreases (↓) when adding (↑) H$_2$</td>
</tr>
<tr>
<td>Fuel Mixture</td>
<td>Equivalence Ratio at 0% O₂</td>
<td>NOₓ [ppmdv]</td>
</tr>
<tr>
<td>------------------------------</td>
<td>----------------------------</td>
<td>-------------</td>
</tr>
<tr>
<td>76% CH₄ - 24% H₂</td>
<td>1.0</td>
<td>↑ 16%</td>
</tr>
<tr>
<td>94% CH₄ - 6% C₂H₆</td>
<td>1.0</td>
<td>↑ 5%</td>
</tr>
<tr>
<td>95% CH₄ - 5% C₃H₈</td>
<td>0.87</td>
<td>↑ 4%</td>
</tr>
<tr>
<td>98% CH₄ - 2% CO₂</td>
<td>0.87</td>
<td>↓ 4%</td>
</tr>
</tbody>
</table>
1 Introduction

Currently, the bulk of energy demand is provided by fossil fuels; see. Figure 1 shows fossil fuel energy consumption as a percentage of the total energy consumption, for the United States and worldwide, and how it has developed for the past three decades. The figure indicates that most energy demand in the US is satisfied with fossil fuels.

![Figure 1: Fossil fuel energy consumption as a percentage of the total consumption, extracted from [1].](image)

This situation is expected to continue for the next few decades, hence the importance of developing near zero emissions technologies that can achieve high efficiency levels while keeping the pollutant emissions at a minimum. Also, it is a goal to satisfy the global energy demand within a sustainable model.

Traditionally, combustion processes are carried out with the oxygen in the air acting as the oxidizer (Oxygen-O₂ is ~ 21\% by volume in air). Oxy-fuel technology uses oxygen enriched air and even pure oxygen as an efficient alternative to reduce NOx emissions and increase the reactions temperature.

1.1 Motivations to use an oxy-fuel burner

The immediate consequences of working with pure oxygen instead of air are the following [2]–[4]:

- Higher flame temperatures: removing nitrogen from the oxidizer results in higher temperatures, since N₂ is an inert gas that consumes heat from the combustion reactions.
- Higher heat transfer rates: In addition to the high temperatures and luminosity, the oxy_fuel technology improves the heat transfer rate. Using pure oxygen instead of air allows a significant reduction of the volume of the flue gases, which implies that the heat used to increase the temperature of the flue gases will be transferred to the bulk furnace gas and walls, instead to the N₂ in the air.
- A small increase in the bulk furnace gas temperature causes a sharp increase in the gas-to-load radiative heat transfer rate due to the strong temperature dependence of radiative heat transfer. This improvement is also caused by the higher concentration of triatomic molecules
(H₂O, CO₂) in the combustion chamber, H₂O and CO₂ transfer radiation heat better than the diatomic molecules (O₂, N₂).

- Low NOₓ emissions: working with pure oxygen will lead to a zero NOₓ scenario, but nitrogen can come from different sources, such as impurities in either the oxygen or the fuel and air leaks. It is known that higher temperatures promote an increase in NOₓ concentration, but if enough O₂ is added in the oxidizer, it will overweight the effect of the increased flame temperature. However, working with oxygen instead of air also means reducing the flue gases volume, thus even if the NOₓ concentration, obtained at high levels of oxygen purity, is higher compared to the air-fired combustion, the amount of NOₓ produced by the oxy-gas combustion would be less due to this reduction of flue gas volume.

- Higher CO₂ concentration in the flue gases that promotes the opportunity to capture it by direct physical compression and cooling techniques.

1.2 Alternative fuels

Natural gas is a relatively clean-burning fuel and is used in many applications. It ranks second to coal in the production of electricity in the United States, being the source of the 27% of the US electricity generation [5]. But concerns over global warming, environmental degradation, and national energy independence have sparked interest in alternative fuels, which could be defined as any fuel that has potential for displacing or supplementing the traditionally used conventional fuels [2].

Actual burner designs commonly allow the interchangeability between a few different fuels, mainly with the purpose to reduce pollutant emissions while maintaining the same efficiency levels or even improve them. Since the burner modelled in this project usually operates with natural gas, three type of different gases comparable with natural gas have been studied:

- **Fuel type 1: Hydrogen enriched natural gas.** Hydrogen is the most abundant element on earth, whose combustion products do not contain greenhouse gases and, in the ideal case of oxy-fuel combustion, only water will be produced. However, current infrastructure does not support hydrogen as a wide-spread fuel. In order to expand the role of hydrogen in the near term, one option is to use hydrogen by mixing it with natural gas [6].

- **Fuel type 2: Landfill/digester biogas.** Biogas is a gaseous product of the anaerobic digestion of organic matter. It is usually composed by methane (50%-80%) and carbon dioxide (20%-50%), along with other trace gases. When processed to higher purity can be used as an alternative fuel for natural gas vehicles [7].

- **Fuel type 3: Mixtures with heavier hydrocarbons.** C₂H₆ and C₃H₈ are commonly found as trace gases in commercial natural gases. These molecules have similar properties than CH₄ due to all belong to the same family: alkanes or paraffin (CₙH₂ₙ₊₂) [2].

2 Key features

For this project the Oxygen fuel burner Eclipse Primefire 300 has been modeled numerically in order to study how the emissions levels vary when changing the fuel type, the concentration of oxygen in the oxidant and the oxygen to fuel ratio. This burner is composed of two nozzles (one nozzle enclosed by the other nozzle). Both nozzle tips are flush with the pre-combustor chamber, which is a ceramic block made of insulating bricks. This same burner was subject to previous testing done at GTI under CEC Contract 500-05-026). Figure 2 shows an isometric draft of the nozzles on the left and a picture of the burner and pre-combustor chamber on the right.
The inner nozzle conducts the fuel stream, whereas the oxidizer passes through the gap between the external walls of the inner nozzle and the internal walls of the outer nozzle. Both streams start mixing at the nozzle tip, where the pre-combustor chamber starts, in order to prevent high heat released. In the pre-combustor length some mixing occurs, however the oxygen stream keeps enveloping the fuel stream up to the entrance of the furnace chamber is reached. The purpose of this pre-combustor is to isolate the metallic burner tip from the radiation of the flame and furnace walls [4].

The burner produces a characteristic flat flame, which volume is increased considerably compared to the traditional round flames, thus improving the heat transfer to the load. Another important characteristic of this burner is that the flame presents a rich zone and a lean zone, referred to the concentration of the oxidizer, fact that promotes the soot creation and destruction in each zone, respectively. The presence of soot increases considerably the flame luminosity. The Eclipse Primefire 400 burner uses this characteristic, and by deviating a little amount of the oxygen to the fuel stream the creation of soot precursors, such as polycyclic aromatic hydrocarbons (PAH) are enhanced and therefore it is increased the flame luminosity. The flame luminosity plays an important role in the process since it is directly related to the radiant heat transfer, which is the main way to transfer heat in the most commons applications of this burner, such as glass melting, aluminum melting, etc. [2]–[4], [8].

### 2.1 Operating conditions

The Eclipse Primefire 300 burner is available for different thermal power ranges. The model studied in this project has been the 2 MM BTU/hr (586 kW). The primarily fuels that are employed for this model are natural gas and liquid petroleum gas (LPG). For the purpose of this project, natural gas has been the baseline for all the cases studied. Table 3 summarizes the operating conditions for the chosen model.

<table>
<thead>
<tr>
<th>Thermal power</th>
<th>586 kW</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel</td>
<td>Natural gas, Fuel type I, II and III</td>
</tr>
<tr>
<td>Oxidizer</td>
<td>Oxygen (99%O₂-1%N₂) mix by volume</td>
</tr>
</tbody>
</table>

The 1% of N₂ impurity presented by the oxidizer is provided by cryogenic ASU technologies capable to reach such high levels of refinement [9], and it has been proved to be enough in order to predict the trends for NOx emissions.
3 Virtual AeroThermal Field - Computational fluid dynamics (CFD)

3.1 Introduction

Burners and furnaces designs have always been a problem that engineers have had to confront. High heat transfer efficiency levels and low emission are the most commonly required features for this type equipment. The important development achieved in computational resources has arisen the use of numerical methods as the main tool to help engineers in this task. Particularly, CFD simulations have been proved to provide accurate results, useful to understand the system performance while saving huge amounts of money, time and effort that would imply to analyze the same case scenarios with prototypes.

One of the aspects of capital importance in burners design consists in minimize the emission of pollutant contributors, such as NOx or CO. Since an accurate description of pollutant formation would require a high number of species and reactions, it is currently impractical to include all phenomena of importance for pollutant formation in a single CFD. Besides that, it is possible to perform a CFD simulation with detailed treatment of fluid dynamics with reduced chemistry, thus obtaining accurate results of fluid flow, the temperature field, heat transfer rates and a first guess for the flow composition, since the pollutant contributors are considered trace species, whose influence in the results for this aspects is of a minor relevance. Then, the output solution of the CFD is used to realize an analysis with a detailed chemistry, being then able to obtain a more accurate solution for the species concentration (including the trace species) through a chemical reactor network (CRN), created upon the CFD results [10], [11]. More information regarding the CRN it is given in Chapter 4.

Details and explanations of the steps followed in order to carry out the CFD simulations are exposed in the following sections of this chapter, as well as a presentation and discussion of the results obtained for different case scenarios. Since the software ANSYS FLUENT 15.0 has been the workhorse for this project, the information is provided following the order as it is required by the program: geometry, mesh, models, boundary conditions and solutions.

3.2 Geometry

When dealing with CFD simulations the volume occupied by the fluid must be modeled, and it is referred as the fluid domain. The entire volume compressed by the fluid domain is shown on the left of Figure 3, whereas on the right side, a section plain with different parts named in order to match the description given in the previous chapter can be observed. Details regarding the dimensions of the model can be found in the Appendix A.
Figure 3: Volume modeled on the left and a section plane with named parts on the right.

The burner nozzle is composed of two different volumes, which correspond to the oxygen flow and the fuel flow. As explained in the previous chapter, both streams reach the pre-combustor where the two streams start mixing. Finally, where the pre-combustor ends, the furnace chamber starts. A square section for the outlet has been chosen rather than a circular one to simplify the meshing process.

Given the symmetry with respect to the top and right planes, only a quarter of the volume, shown in Figure 3, has been modeled, being able then to achieve high levels of mesh refinement, and therefore a more accurate solution, while keeping the CPU load at a reasonable levels. Thus, the geometry that has been finally created with the ANSYS Design Modeler [12], and the starting point for further steps, is the one presented on Figure 4.

3.3 Mesh

To proceed and solve the problem it is necessary to divide the fluid domain into small cells, also referred as elements, with the purpose of treat each element as a single control volume where the suitable set of
equations are solved. The solution of each cell, as well as the error, are transferred to the neighboring elements in each iteration, until the convergence criteria is met. Obviously, the amount of either computational time or computational resources needed to reach the solution increases with the number of cells, but also a more accurate solution is achieved, thus the importance of creating an efficient and reliable mesh.

3.3.1 Approach

In order to achieve the goals posed before, it has been proceeded to divide the fluid domain into different blocks, each one representing different zones of interest, enabling then to have high levels of refinement on those zones where smaller elements are needed to reach enough accuracy. Also, the subsequent blocks created are prisms, allowing then the sweep method of the ANSYS Workbench Mesher, which means that the mesh will be composed of hexahedral cells, which are quite more efficient than the otherwise employed tetrahedral cells [13]. The divided domain is shown in Figure 5, which precedes the consequent brief description of each block.

![Figure 5: Fluid domain divided into blocks.](image)

The block 1 represents the burner nozzle, followed by the pre-combustor chamber showed as block 2. The centerline of the pre-combustor, which is the zone where the flame is going to exist, is represented by the blocks number 3 and 4, being number 3 the core of the flame and number 4 the bulk of the combustion productions. Blocks 5 and 6 are intended as the surrounding of blocks 3 and 4, respectively. As it may seem logic, blocks numbered from 1 to 4 are those with a smaller element size and therefore the refined zones, whilst a larger element size is used on the remaining blocks.

3.3.2 Mesh sensitivity analysis

To confirm that a converged model solution is mesh independent, it is necessary to carry out a mesh sensitivity analysis. It consists on running the same models and boundary conditions within more refined and coarser meshes, then compare the results and finally select the mesh with the least amount of elements that provides good results.

3.3.2.1 Mesh quality

The mesh quality plays a significant role in the accuracy and stability of the numerical solution, hence the importance of checking the quality of the mesh before running the solver. To achieve a fair sensitivity analysis it is necessary to make the comparison between meshes within reasonable quality intervals. The quality indicators checked during this analysis are the following:

- **Orthogonal quality**: the worst cells will have an orthogonal quality closer to 0, with the best cells closer to 1. The minimum orthogonal quality for all types of cells should be more than 0.01, with an average value that is significantly higher.
• **Aspect ratio**: is a measure of the stretching of the cell. Generally, it is best to avoid sudden and large changes in cell aspect ratios in areas where the flow field exhibit large changes or strong gradients.

The values provided by *Fluent 15.0* are therefore the minim value for the orthogonal quality and the maximum for the aspect ratio. More information regarding the equations used to compute the value of the indicators can be found in the *Fluent User’s Guide* [14]. Table 4 summarizes the important features for the different meshes that have been created and tested: the number of elements, the minim orthogonal quality and the maximum aspect ratios. The differences between the quality indicators for the different meshes are insignificant, being thus the solution only dependent on the level of refinement.

<table>
<thead>
<tr>
<th>Name of the Mesh</th>
<th>Number of elements</th>
<th>Minimum orthogonal quality</th>
<th>Maximum aspect ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>M1</td>
<td>850741</td>
<td>0.3045</td>
<td>13.79</td>
</tr>
<tr>
<td>M2</td>
<td>1130452</td>
<td>0.3045</td>
<td>13.79</td>
</tr>
<tr>
<td>M3</td>
<td>1305806</td>
<td>0.3399</td>
<td>16.47</td>
</tr>
<tr>
<td>M4</td>
<td>1697303</td>
<td>0.3399</td>
<td>16.47</td>
</tr>
<tr>
<td>M5</td>
<td>2271395</td>
<td>0.2695</td>
<td>17.02</td>
</tr>
</tbody>
</table>

Meshes M1 and M2 have the same level of refinement for the blocks that compose the centerline of the domain (blocks number 1 to 4), differenced only by the element size of the surrounding blocks (blocks 5 and 6), and here lies the reason why they have the same quality indicators. This same characteristic is found in meshes M3 and M4, whose centerline is more refined compared to the previous meshes. Finally, mesh M5 is the one that presents the higher refinement on the centerline blocks and the surroundings.

The models, boundary conditions and the approach employed in this analysis are presented in further sections of this Chapter 3, since they have been also used for the rest of the studied cases. In order to compare the results, the temperature profile for the z axis has been used, since it is the centerline of the fluid domain and the zone where the flame lies.

3.3.2.2 **Sensitivity analysis results**

Figure 6 shows the centerline temperature profile of the converged solution for each mesh.
As it can be observed, meshes with the same level of refinement of the centerline blocks present basically the same profile, regardless of the refinement of the surrounding blocks. Meshes with the poorest levels of refinement (M1 and M2) yield to a solution that differs significantly when compared to the more refined meshes, whereas the difference between meshes M3, M4 and M5 are considered to be negligible, since the maxim temperature and the position where it is reached and the outlet temperature are essentially equal for the three cases, proving then that a mesh independent solution has been reached. Thus, the selected mesh has been the one named as M3, since it is the one that provides an accurate, stable and reliable solution, in a more efficient manner (referred to the computational time needed to reach the solution). Figure 7 shows an isometric view of the M3 mesh.
3.4 Models

Table 5 is an overview of the solver set up and the models used for the cases studied. Information about the governing equations and its parameters can be found in the ANSYS FLUENT User’s Guide [14].

<table>
<thead>
<tr>
<th>Solver</th>
<th>Steady</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Pressure based</td>
</tr>
<tr>
<td></td>
<td>3D case</td>
</tr>
<tr>
<td>Pressure-velocity coupling</td>
<td>Simple</td>
</tr>
<tr>
<td>Energy equation</td>
<td>On</td>
</tr>
<tr>
<td>Viscous model</td>
<td>Realizable $\kappa$-$\varepsilon$</td>
</tr>
<tr>
<td></td>
<td>Enhanced wall treatment</td>
</tr>
<tr>
<td>Radiation model</td>
<td>Discrete Ordinates (DO)</td>
</tr>
<tr>
<td>Species model</td>
<td>Partially Premixed Model</td>
</tr>
</tbody>
</table>

The Realizable $\kappa$-$\varepsilon$ is an update of the Standard $\kappa$-$\varepsilon$ to model flow turbulence; it provides more accurate solutions than Standard $\kappa$-$\varepsilon$. To model the radiation heat transfer, the Discrete Ordinates (DO) model has been selected over the P-1 model. The latter tends to over predict the radiation heat transfer rate, especially in problems with high temperatures, which is the case of the oxy-gas flame. Since the oxidant and fuel streams are not premixed and there is some level of premixing in the pre-combustor section; for the species model the Partially Premixed Model has been selected and coupled with the Zimont model [15] to calculate the turbulent flame speed.
3.5 Boundary conditions

A list of the boundary conditions and their type can be found in Table 6. A more detailed description of each boundary can be found in the upcoming subsections and in the Appendix A.

<table>
<thead>
<tr>
<th>Boundary name</th>
<th>Boundary type</th>
<th>Value [unit]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fluid domain</td>
<td>Interior</td>
<td>----</td>
</tr>
<tr>
<td>Fuel inlet</td>
<td>Mass flow rate inlet</td>
<td>Variable=f(heat_input, fuel class)</td>
</tr>
<tr>
<td>Oxidizer inlet</td>
<td>Mass flow rate inlet</td>
<td>Variable=f(heat_input, fuel class, excess of oxidant)</td>
</tr>
<tr>
<td>Outlet</td>
<td>Pressure outlet</td>
<td>P=0 gauge; See Appendix A</td>
</tr>
<tr>
<td>Chimney wall</td>
<td>Wall</td>
<td>Adiabatic</td>
</tr>
<tr>
<td>Brick walls</td>
<td>Wall</td>
<td>Water cooled; see Appendix A  for details</td>
</tr>
<tr>
<td>Pre-combustor</td>
<td>Wall</td>
<td>See Appendix A for details</td>
</tr>
<tr>
<td>Outer oxygen walls</td>
<td>Wall</td>
<td>See Appendix A for details</td>
</tr>
<tr>
<td>Inner oxygen walls</td>
<td>Wall</td>
<td>See Appendix A for details</td>
</tr>
<tr>
<td>Fuel walls</td>
<td>Wall</td>
<td>See Appendix A for details</td>
</tr>
<tr>
<td>Symmetric planes</td>
<td>Symmetry</td>
<td></td>
</tr>
</tbody>
</table>

3.6 Solution Methods

The procedure followed for all the simulations is presented below:

- For the first 1000 iterations, the default methods were used; the Green Gauss Node was chosen to evaluate the gradients and derivatives. This is due to the increased accuracy of the method relative to the less computationally expensive Green-Gauss cell based method as discussed by ANSYS INC. [14].
- For the following 9000 iterations, the second order upwind discretization method has been used to solve all the equations. Second order discretization is better able to resolve curvature and gradients than the first order discretization scheme.

This approach has always lead to a solution that meets all the requirements to accept it as a converged solution. This requirements are explained in the next section.

3.7 Convergence criteria

The following conditions are required to consider a solution to be converged:

- Stabilized residual plot: all the residuals must be stabilized at the end of the simulation at reasonable low values.
- The unbalanced mass flow rate of the system, which is given by the difference between the sum of the inlet mass flow rates and the outlet mass flow rated, must be less than 1% of the total input (sum of the oxidizer mass flow rate and the fuel mass flow rate).
The unbalanced heat transfer rate, which is calculated by the difference between the heat of the reaction source and the heat lost through the outlet and the walls, must be less than 1% of the total input, which is the thermal power with a fixed value of 586 kW.

Figure 8 along with Table 7 and
Table 8 serve as an example of how the residuals plot should look like and examples of acceptable mass and heat flux reports, respectively. All the examples given correspond to the reference case: fuel mixture of 100% CH₄ and stoichiometric conditions.

![Figure 8: Residuals plot.](image)

Table 7: Mass flow rate report.

<table>
<thead>
<tr>
<th></th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel inlet</td>
<td>0.002927 kg/s</td>
</tr>
<tr>
<td>Oxygen inlet</td>
<td>0.011782 kg/s</td>
</tr>
<tr>
<td>Outlet</td>
<td>-0.014709111 kg/s</td>
</tr>
<tr>
<td>Net</td>
<td>-1.1315569e-07 kg/s</td>
</tr>
<tr>
<td>% of the total input</td>
<td>0.00077 %</td>
</tr>
</tbody>
</table>
4 Chemical reactor network (CRN)

The emissions from the burner are subject to regulations strict regulations, and more stringent regulations are foreseen. These reasons make the capability of predicting pollutant emissions a valuable tool during the design phase or to predict in the field the impact of the fuel composition on emissions and stability, and make decisions accordingly. Instead of building prototypes, this strategy allows to make informed decisions previous to the construction of the prototype and thus avoiding the waste of economic resources.

Obtaining a detailed prediction of minor species, such as pollutant or harmful species (like NOx or CO), requires a detailed chemistry set; i.e. GRI 3.0 [20], UC San Diego mech [21], USC mech II [22]... , which are not included in the CFD simulations; in general, the computation cost of the chemical reactions is more expensive than the computation of the fluid dynamics equations. However, main flame properties like temperatures, heat release, velocities and main species can be well predicted using a simplified kinetics mechanism. The output solution of the CFD simulation is used afterwards to construct an equivalent reactor network of ideal chemical reactors, and the concentration of minor species is calculated using a detailed chemical scheme. Therefore, the equivalent reactor network becomes the basis for high-fidelity kinetics simulation, while maintaining spatial information derived from the CFD model. For all the cases the reaction mechanism employed has been the GRI 3.0 [20].

4.1 Zonal distribution

Several methods have been proposed with the objective to achieve an equivalent reactor from the CFD solution obtained with a simplified chemical scheme [10], [23]. The new release ANSYS FLUENT 15.0 incorporates an option that allows the user to automatically generate an equivalent reactor network from a converged CFD solution. The user can select the number of reactors to fill the fluid domain.
Being the grid of CFD and its solution the starting point, the first step consists in agglomerating the CFD cells into the specified number of reactors. For optimal performance, CFD cells grouped together in each reactor have temperatures and species mass fractions that are similar. For the partially premixed model, the cell temperature and the cell mixture fraction are employed to cluster the cells in different reactors, until the final number of reactors is reached. Finally, the species concentration in each reactor is calculated using the detailed chemical scheme, thus providing more information regarding the minor species [24]. Since the CRN is a postprocessor strategy, a precise solution of the pollutant species requires an accurate CFD solution. The CRN results are only good if the solution obtained with the CFD strategy alone is accurate.

4.2 Reactor network sensitivity analysis

The equivalent reactor network generated consists of the defined number of reactors defined by the user, where every reactor is modeled as with a Perfectly Stirred Reactor (PSR) at fixed temperature (Temperature solution from CFD results). This fact becomes of capital importance when selecting the number of reactors for the network. In order to reach a solution independent from the number of reactors, a sensitivity analysis is carried out. The idea is to increase the number of reactors in the network and then check the results independence to this variable. For The sensitivity analysis the mass fraction of NOx and CO were checked. Once the minimum number of reactors necessary to reach an accurate and mesh independent solution has been decided, that number is fixed for the different runs and only excess of oxidant is varied. The default settings for the calculation have been left default; only the maximum number of iterations has been increased to guarantee similar residual values.. The reactor pressure is fixed and determined as the mass averaged pressure of the CFD cells conforming the reactor [24].

Figure 9 and Figure 10 show the sensitivity of NO and CO results to the number of reactors for 100% CH₄ and operating at stoichiometric conditions. The mass fractions of the species are measured at the stack outlet. For 550 reactors or more, the results become insensitive to this variable.

![Figure 9: NO mass fraction vs. Number of reactors for 100% CH₄.](image)
As it can be observed, a high number of reactors are required in order to reach an independent. A large number of reactors is required to provide a spatial resolution of the chemical reactions.

Analyzing the results of Figure 10, it can be seen that for the CO mass fraction the solution seems to be stabilized when using more than 200 reactors, whilst the NO mass fraction needs more than 500 reactors to reach a stable value. For some cases an upper limit of 700 reactors was found. For those cases, it was not possible to create a network of 700 reactors or more due a recurrent error during the iterative process to solve the network equations. The sensitivity analysis for other fuel types are collected in Appendix B.

Another remarkable point to account for in this analysis is the time required to reach the solution. Figure 11 shows the increase of the computational time needed when increasing the number of reactors of the network.
As it is shown, the computational time increases in a considerably manner when increasing the number of reactors of the network. Here lays the importance to select the proper number of reactors with the goal to maintain the overall efficiency of the simulation (referred to computational time needed) at a reasonable level.

5 Results and Discussion

The fuel mixtures studied in this project are summarized in Table 9. The baseline fuel is 100% CH4.

Table 9: Studied fuel mixtures.

<table>
<thead>
<tr>
<th>Fuel type 1 (hydrogen enriched natural gas)</th>
<th>Fuel type 2 (Biogases)</th>
<th>Fuel type 3 (mixtures with heavier Alkanes)</th>
</tr>
</thead>
<tbody>
<tr>
<td>80% CH4-20% H2</td>
<td>96% CH4-4% CO2</td>
<td>85% CH4-15% C2H6</td>
</tr>
<tr>
<td>50% CH4-50% H2</td>
<td>60% CH4-40% CO2</td>
<td>75% CH4-25% C2H6</td>
</tr>
<tr>
<td>40% CH4-60% H2</td>
<td>55% CH4-45% CO2</td>
<td>75% CH4-25% C3H8</td>
</tr>
<tr>
<td>30% CH4-70% H2</td>
<td>45% CH4-55% CO2</td>
<td>75% CH4-15% C2H6-10% C3H8</td>
</tr>
</tbody>
</table>

For each fuel mixtures, the global equivalence ratio is varied within the following values: 1, 0.9, 0.8 and 0.5, with the goal to study the effect of operating in fuel lean conditions. In sharp contrast with the premixed flames cases, a stability analysis is not needed due to the high stability of the diffusion flames. Thus in the results obtained at very lean conditions (equivalence ratio equal to 0.5) no blow off instabilities have been observed, with the exception of the fuel type 2 mixtures, whose limits will be
explained in its own section. Finally, the upcoming sections present first the results obtained directly from the CFD simulations and afterwards the results provided by the reactor network solution.

5.1 Fuels type 1: Hydrogen enriched natural gas

5.1.1 CFD results

Figure 12 presents the maximum temperature (at stoichiometric conditions) as function of the volumetric percentage of H₂ in the fuel mixture.

As it can be observed, the maximum temperature increases when adding hydrogen to the mixture. This trend is inagreement with the trend obtained with the equilibrium calculation done with the CHEMKIN PRO software [25], which can be found in the Appendix C.

Figure 13 to Figure 17 show the temperature contour of the horizontal symmetric plane for the different type 1 mixtures presented on Table 9, fired at stoichiometric conditions.
Figure 13: 100% CH₄ temperature contour.

Figure 14: 80% CH₄-20% H₂ temperature contour.
Figure 15: 50% CH₄-50% H₂ temperature contour.

Figure 16: 40% CH₄-60% H₂ temperature contour.
It is clear the variation of the temperature profile for the different mixtures. Working with mixtures with high content of hydrogen leads to shorter and narrower flames due to the high reactivity of the hydrogen, fact that will affect the emissions as discussed in the next subsection.

The effect of operating at lean conditions is presented in Figure 18 and Figure 19, which represent the variation of the exhaust gases temperature and the heat transferred to the walls, respectively, when varying the equivalence ratio. No clear trends have been detected regarding the maximum temperature reached when varying the equivalence ratio. Since the maximum temperature is the value of a single cell, it is not representative of the overall system; besides diffusion flames naturally displays regions where the equivalence ratio leads to peaks of maximum temperature.
It can be concluded that operating at lean conditions decreases the overall efficiency of the process. Lower exhaust temperatures are obtained due to the increase of the total mass flow input. Also, the heat released from the reaction is used to heat up the increased amount of flue gases, thus less heat is transferred to the load. The heat transferred to the load seems to be insensitive to the addition of hydrogen to the fuel mixture.

5.1.2 CRN results

Figure 20 and Figure 21 are representative of the effect of both equivalence ratio and fuel mixture on the main species concentration: H₂O and CO₂, which are the main combustion products.
The excess of oxygen inherent of the lean conditions contributes to the dilution of the product gases, being then the molar concentration obtained for both species lower at lean conditions. On the other hand, the effect of hydrogen addition to the fuel mixtures leads to higher concentrations of H$_2$O and a reduction of the CO$_2$ molar fraction. These results can be easily explained once the stoichiometric balance of the combustion reaction of Equation 7 is done. Despite its simplicity, these results become useful when discussing the results for the minor species.

\[
\alpha \cdot CH_4 + (1 - \alpha) \cdot H_2 + \frac{(3\alpha + 1)}{2} \cdot O_2 \rightarrow \alpha \cdot CO_2 + (\alpha + 1) \cdot H_2O
\]

*Equation 1: CH$_4$-H$_2$ stoichiometric balance.*
5.1.2.1 NOx emissions

The NOx predictions are presented through Figures 22 to 24. Different points of view regarding the units to measure NOx have been used. First of all, Figure 22 shows the trends in form of NOx concentration in ppmdv (dry basis and corrected to 0% O2), whereas Figures 23 and 24 represent the NOx trends in terms of emission index; the difference between them is the variable used to normalize the NOx production rate: the emission index from Figure 23 is measured in gNOx/kgFuel_burned while Figure 24 is given in mgNOx/kWh_fuel burned. The measured NOx at the outlet is plotted against the equivalence ratio for all the different fuel mixtures. Previous studies using a similar burner (CEC Contract 500-05-026) operated on natural gas at 0% excess O2 yielded NOx emissions between 1500 and 3000 ppmvd. These burners tend to operate near an equivalence ratio of 1.0. Hence the results obtained from the CRN as shown in Figure 22 are of the same order, which is encouraging. Furthermore, the trends obtained have been compared with the ones obtained with the equilibrium calculation (see Appendix C) and have result to be in good agreement.

Figure 22: NOx emissions in ppmdv @ 0% O2 vs. equivalence ratio for all type 1 mixtures.
The following key points summarize the behavior of NOx emissions for the different type I fuel mixtures:

- For a fixed equivalence ratio, the addition of hydrogen yields to an increase of NOx concentration, mainly due to the higher temperatures that are reached with mixtures with high content of hydrogen. The most important route to form NOx in oxy-fuel combustion is the thermal or Zeldovich route, whereas the Fenimore or prompt route becomes important due to the negative net production rates of NOx [26], [27]. Also the addition of H₂ enhances the formation of intermediate species like OH and H, which promotes NOx formation through the Zeldovich, NNH and N₂O pathways.
The thermal route is enhanced by the addition of H\textsubscript{2} since the mechanism is comprised of the three following reactions: N\textsubscript{2} + O = N + NO; N + O\textsubscript{2} = NO + O; and N + OH = NO + H.

The NNH reactions enhanced include NH + N = N\textsubscript{2} + H; NH + NO = N\textsubscript{2} + OH; NNH + M = N\textsubscript{2} + H + M; NNH + O\textsubscript{2} = HO\textsubscript{2} + N\textsubscript{2}; NNH + O = OH + N\textsubscript{2}; NNH + H = H\textsubscript{2} + N\textsubscript{2}; NNH + OH = H\textsubscript{2}O + N\textsubscript{2}; and NNH + CH\textsubscript{3} = CH\textsubscript{4} + N\textsubscript{2}.

The reactions that explain the effect of hydrogen addition on the N\textsubscript{2}O intermediate mechanism are the following: O + N\textsubscript{2} + M = N\textsubscript{2}O + M; N\textsubscript{2}O + H = NO + NH; O + N\textsubscript{2}O = NO + NO.

Also the high availability of O\textsubscript{2} in the oxidant increases the concentration of O-atoms, which also participates in all NOx formation pathways.

- At a fixed equivalence ratio the addition of hydrogen affects the flame length and width, the flame becomes shorter and narrower with the addition of hydrogen to the fuel mixture. Shorter flames yield to less recirculation of the product gases into the reaction zone, which also explains the increase in NOx concentration.

For all the fuel mixtures, operating at fuel lean conditions leads to a considerable increase of the NOx production, conversely to what happens in air-fired flames. As it is shown by the equilibrium calculations regarding the equivalence ratio effect for oxygen and air cases (see Appendix C), the excess of oxygen does not decrease the flame temperature as it happens with the excess of air. Increasing then the amount oxygen used means increasing the amount of N\textsubscript{2} entering the chamber, since the oxidizer is assumed to have 1% of N\textsubscript{2}. High temperatures together with higher amount of N\textsubscript{2} lead directly to a considerable increase of NOx production. The results discussed before are based on NOx concentration by volume, while the emission index (EINOx) sheds light on the NOx production on a mass basis. When comparing the EINOx for the different mixtures, the differences become less pronounced, but still exist. This is due to the increased amount of water produced when adding hydrogen to the combustion (it can be seen in Figure 24), once water is drop out of the system the dry emissions are shifted upwards virtually indicating a higher concentration (ppm\textsubscript{NOx\_dry\_basis}>ppm\textsubscript{NOx\_wet\_basis}). For hydrogen containing fuels, the virtual shift caused by drying the sample, is significant.

### 5.1.2.2 CO emissions

The CO predictions, using the same units of measure used for NOx, are shown in Figures 25, 26 and 27. Again, results from the GTI studies (CEC Contract 500-05-026), indicate CO levels from 300 to 1000 ppmvd at 0% O\textsubscript{2}. The levels from the CRN are somewhat higher, especially at stoichiometric conditions, but the overall magnitudes are similar. Also, comparison with equilibrium calculations (see Appendix C) have proved to be in good agreement.
Figure 25: CO emissions in ppmdv @ 0% O₂ vs. equivalence ratio for all type 1 mixtures.

Figure 26: EICO in gNOx/kgFuel vs. equivalence ratio for all type 1 mixtures.
The following key points serve to explain the trends and behavior of the predicted CO:

- High levels of CO are obtained due to the high temperatures reached in oxy-fuel combustion, since it contributes to the dissociation of CO₂ molecules into CO and O-atoms.
- Due to its own nature, diffusion flames present local zones where the combustion is produced at overly fuel-lean or overly fuel-rich conditions, being both situations responsible of a not complete combustion [2], [27].
- For all the fuel mixtures, all the CO indices are triggered to very high values near at the stoichiometric point (equivalence ratio = 1). These high levels of CO can be explained by combining the fact that CO is generally produced by the incomplete combustion of carbon containing fuels and the high temperatures (that also promote the CO production) reached in oxy-fuel cases. When working at lean condition, the excess of oxygen helps to complete combustion process and thus lowering considerably the CO emissions.
- The addition of hydrogen to the fuel reduces the emission of carbon monoxide, as it is better represented by Figure 27. Again, the higher reactivity of hydrogen helps to complete the oxidation reactions avoiding incomplete combustion products. Moreover, the additional hydrogen acts displacing carbon from the fuel, so inherently less CO can be formed.

5.2 Fuels type 2: Landfill/digester biogas

5.2.1 CFD results

Figure 28 illustrates the effect that the addition of CO₂ causes on the maximum temperature reached in the flame, which has been obtained from the CFD simulation, for the stoichiometric point.
The maximum temperature decreases drastically with the addition of CO₂ to the fuel mixture, as shown in Figure 28. This is due to the role that CO₂ plays in the fuel: it acts only diluting the mixture. Therefore, the amount of CO₂ needs to be heated up, and the flame temperature will be lowered consequently. This drop of the flame temperature will affect the pollutant emissions, as it will be discussed in the next subsection. The same trend has been obtained with the equilibrium calculation (see Appendix C) [25].

Figures 29 to 33 show the temperature contour for the different concentrations of CO₂ in the fuel mixtures presented on Table 12, fired at stoichiometric conditions.
Figure 29: 100% CH$_4$ temperature contour.

Figure 30: 96% CH$_4$-4% CO$_2$ temperature contour.
Figure 31: 60% CH₄-40% CO₂ temperature contour.

Figure 32: 55% CH₄-45% CO₂ temperature contour.
Fuel bends with high content of CO₂ tend to behave like premixed flames. Figures 34 and 35, which show the OH mass fraction of the horizontal plane for the 100% CH₄ and 60%CH₄-40%CO₂ cases, are useful to compare the difference between the two cases: the 100% CH₄ case presents a larger zone with higher gradients of OH as seen in diffusion flames, whereas the 60%CH₄-40%CO₂ case has a smaller zone with more uniform contour of OH typical from the premixed flames.
Figure 34: OH mass fraction contour for the 100% CH₄ case.

Figure 35: OH mass fraction contour for the 60% CH₄-40% CO₂ case.
Because of the premixed-flame behavior of the fuel mixtures with higher levels of CO$_2$, a lean limit has been detected due to the irregular residual plot that the CFD solution presented, and also because it was found impossible to solve the reactor network. Table 13 indicates the lean blow off limit for these mixtures, in terms of the leanest equivalence ratio reachable.

<table>
<thead>
<tr>
<th>Fuel Mixture</th>
<th>Lean Blow Off Limit</th>
</tr>
</thead>
<tbody>
<tr>
<td>60% CH$_4$-40% CO$_2$</td>
<td>0.75</td>
</tr>
<tr>
<td>5% CH$_4$-45% CO$_2$</td>
<td>0.8</td>
</tr>
<tr>
<td>45% CH$_4$-55% CO$_2$</td>
<td>0.95</td>
</tr>
</tbody>
</table>

*Table 10: blow off limit for mixtures with high content of CO$_2$.  

The variation of the exhaust temperature and the heat transferred to the bricks are presented through Figures 36 and 37, respectively.

*Figure 36: Flue gases temperature vs. equivalence ratio for all type 2 mixtures.*
It becomes clear that the addition of CO₂ to the fuel mixture affects the exhaust temperature and the heat transferred to the walls, both variables are reduced when increasing the CO₂ in the fuel mixture. The added CO₂ acts as a heat sink thus lowering the flame temperature, decreasing the exhaust temperature and reducing the heat transferred to the brick walls.

Regarding the effect of working at lean conditions, for the fuel mixtures with high content of CO₂ the temperature of the flue gases seems to maintain around the same value, being not representative of what is expected. However, the decrease of the heat transferred to the bricks at lean conditions indicates that part of the heat released through the reaction has been employed to heat up the larger amount of product gases instead of being transferred to the bricks.

5.2.2 CRN results

Starting again with the molar concentration at the exhaust of the main products of the combustion, H₂O and CO₂, Figures 38 and 39 present the concentration of these species against the equivalence ratio, distinguishing the different fuel mixtures.
Once more, the excess of oxygen inherent to lean conditions dilutes the products since it is not needed to combust, lowering then the concentration of both $H_2O$ and $CO_2$. Figures 38 and 39 also show the effect $CO_2$ addition on these major species: increasing the content of $CO_2$ leads to lower concentrations of $H_2O$ while increases the concentration of $CO_2$, as it can be expected once the stoichiometric balanced of Equation 8 is done.

$$\alpha \cdot CH_4 + (1 - \alpha) \cdot CO_2 + (1 + \alpha) \cdot O_2 \rightarrow 1 \cdot CO_2 + 2\alpha \cdot H_2O$$

Equation 2: $CH_4$-$CO_2$ stoichiometric balance.
5.2.2.1 NOx emissions

Figures 40, 41 and 42 show the NOx trends using the different measurement units that have been seen before: the NOx concentration in ppm (dry basis and corrected at 0% O2), the emission index in gNOx/kgFuel and the emission index expressed in mgNOx/kWh. The measured NOx at the exhaust is plotted against the equivalence ratio for all the different fuel mixtures., the trends obtained have been found to be the same that the ones obtained with the equilibrium calculations (see Appendix C).

![Figure 40: NOx emissions in ppmdv @ 0% O2 vs. equivalence ratio for all type 2 mixtures.](image1)

![Figure 41: EINOx in gNOx/kgFuel vs. equivalence ratio for all type 2 mixtures.](image2)
The behavior of NOx emissions is explained through the following points:

- For a fixed equivalence ratio, the addition of CO\textsubscript{2} to the fuel mixture reduces the concentration of NOx produced, as it can be seen in Figures 40, 41 and 42. As discussed before, the thermal or Zeldovich route becomes the main pathway to NOx creation at temperatures above 1800 K [2]. This temperature is exceeded in all the type 2 mixtures due to the effect of replacing combustion air with oxygen. Since the Zeldovich route depends strongly on the flame temperature, the reduction of it achieved with the addition of CO\textsubscript{2} to the fuel mixture yields to a significant drop of the produced NOx. Also, the increased amount of CO\textsubscript{2} depletes the formation of radicals such as OH, which are essential for the intermediate reactions that compose NOx routes.

- The variation of the type of flame obtained, Non premixed for the undiluted fuel and transitioning increasing the premixing levels when adding CO\textsubscript{2} to the fuel mixture also affects the NOx production. The more uniform contours of the OH concentration and temperatures that are achieved with premixed flames, yield to a NOx reduction.

- The effect of operating with excess of oxygen is clearly shown by Figures 40, 41 and 42: the NOx production is triggered at lean conditions. The temperature variation with the excess of oxygen seems insignificant compared to the increase of the N\textsubscript{2} input that comes with the increased amount of oxidizer entering the burner, which is also primordial to the NOx formation.

- The differences between the fuel mixtures become less sharp when analyzing the emission index in terms of mgNOx/kWh (Figure 42). Since the CO\textsubscript{2} present on the mixture acts diluting the products, the NOx concentration (Figure 40) decreases drastically due to the diluting effect of CO\textsubscript{2}. The marked differences that the emission index expressed in gNOx/kgFuel presents (Figure 41) can be explained by the fact that in order to achieve the same thermal power, the amount of fuel to be burnt increases along with the content of CO\textsubscript{2} in the fuel, since it only acts diluting the mixture.
5.2.2.2 CO emissions

Results for CO are shown in Figures 43, 44 and 45. Again, different terms have been used to analyze the CO$_2$ effect on the CO emissions. See equilibrium calculations in Appendix C.

**Figure 43:** CO emissions in ppmdv @ 0% O$_2$ vs. equivalence ratio for all type 2 mixtures.

**Figure 44:** EICO in gCO/kgFuel vs. equivalence ratio for all type 2 mixtures.
Figure 45: EICO in mgCO/kWh vs. equivalence ratio for all type 2 mixtures.

Figure 46 presents the same data as Figure 45, but only for the cases with higher content of CO₂ on the fuel mixture: 60% CH₄- 40% CO₂, 55% CH₄-45% CO₂ and 45% CH₄-55% CO₂; in order to achieve a better understanding of the CO₂ effect on the CO emissions.

The following key points serve to explain the trends and behavior of the predicted CO:

- At the same equivalence ratio, the dilution of CH₄ with CO₂ yields to a decrease on the production of CO. The decrease on the flame temperatures that comes with the mixtures with high content of CO₂ yields to a decrease of the CO production since its formation pathways depend strongly on the temperature [28].
• Also, since the addition of CO₂ leads to the obtainment of pre-mixed flames, the local zones that present overly rich conditions, which promote the CO production are eliminated and thus the CO emissions are lowered [2].

• For all the fuel mixtures, the CO levels are triggered when reaching the stoichiometric point. Working in slightly lean conditions helps to complete the combustion reactions and therefore the CO is reduced since its formation is related to the incomplete combustion of the carbon containing fuels [2].

5.3 Fuels type 3: Mixtures with heavier hydrocarbons

5.3.1 CFD results

Figure 47 gathers the effect of the fuel composition on the maximum temperature of the solution obtained with the CFD simulations (at stoichiometric conditions). Each line represents the different type 3 fuel mixtures, whereas the horizontal axis corresponds to the content of percentage of CH by volume in the fuel blend.

![Temperature vs. CH₄ in volume](image)

*Figure 47: Maximum temperature vs. % of CH₄ in volume, for type 3 mixtures.*

It can be seen that slightly higher temperatures are obtained when increasing the content of heavier hydrocarbons in the fuel mixture. Specially, the highest temperature has been reached with mixtures with larger amount of C₃H₈ present on the fuel mixture.

Figures 48 to 52 show the temperature profile of the different mixtures provided by the CFD, at the stoichiometric point.
Figure 48: 100% CH₄ temperature contour.

Figure 49: 85% CH₄-15% C₂H₆ temperature contour.
Figure 50: 75% CH₄-25% C₂H₆ temperature contour.

Figure 51: 75% CH₄-25% C₃H₈ temperature contour.
No significant changes on the flame shape and characteristics have been detected. Only a slight decrease of the flame shape when increasing the content of heavier hydrocarbons. It can be concluded that comparable temperatures and profiles have been obtained due to the similar properties of the molecules that conform the different mixtures.

The effect that operating at lean conditions has on the exhaust temperatures and the heat transferred to the brick walls is presented through Figures 53 and 54.
The excess of oxygen acts as a heat sink of cooling the gases down and reducing the heat transfer to the bricks. The effect of the fuel composition on the heat transfer is negligible, mainly due to the similar properties that the different molecules composing the fuel and atmosphere in the combustion chamber.

5.3.2 CRN results

The results obtained for the main products of the combustion reaction, $\text{H}_2\text{O}$ and $\text{CO}_2$, are presented in Figures 55 and 56, in which the molar fraction of these species can be found plotted against the equivalence ratio, for all the type 3 mixtures.
As it has been discussed in the other sections regarding the different types of fuels, the excess of oxygen characteristic of lean combustion acts diluting the concentration of both species. Figures 55 and 56 also show an increase of the CO₂ concentration and a decrease of the H₂O molar fraction that comes with the mixtures that have higher content of heavier hydrocarbons. This fact can be explained with the stoichiometric balance of the reaction, see equation 9.
\[ \alpha \cdot CH_4 + \beta \cdot C_2H_6 + \gamma \cdot C_3H_8 + \frac{(4\alpha + 7\beta + 10\gamma)}{2} \cdot O_2 \rightarrow (\alpha + 2\beta + 3\gamma) \cdot CO_2 + (2\alpha + 3\beta + 4\gamma) \cdot H_2O \]

**Equation 3:** \( CH_4 \cdot C_2H_6 \cdot C_3H_8 \) stoichiometric balance.

### 5.3.2.1 NOx emissions

Figures 57, 58 and 59 present the results obtained for the NOx in the form of concentration in ppm (dry basis and corrected at 0% \( O_2 \)), emission index in gNOx/kgFuel and the emission index expressed in mgNOx/kWh, respectively.

![Figure 57: NOx emissions in ppmdv @ 0% \( O_2 \) vs. equivalence ratio for type III mixtures.](image1)

![Figure 58: EINOx in gNOx/kgFuel vs. equivalence ratio for all type 3 mixtures.](image2)
The following key points summarize the behavior of NOx emissions for the different type III fuel mixtures:

- As it can be observed in all the Figures, the results for the different mixtures are collapsed around the same values, again due to the similarities of the different fuels. However, the NOx emissions of the 75% CH₄-25% C₃H₈ seem to be slightly higher, thus indicating the temperature dependence of the NOx formation.
- It is clear that the excess of oxygen affects increasing the NOx emissions, as it has been found for all the fuel types. The increased amount of the oxidizer mass flow entering the chamber does not lower the temperatures enough to counteract the larger amount of N₂ that comes with it, thus resulting the NOx emissions triggered at lean conditions.

5.3.2.2 CO emissions

The CO predictions using the same terms that have been employed before are presented in Figures 60, 61 and 62.
**Figure 60:** CO emissions in ppmvd @ 0% O₂ vs. equivalence ratio for all type 3 mixtures.

**Figure 61:** EICO in gNOx/kgFuel vs. equivalence ratio for all type 3 mixtures.
The following key points serve to explain the trends and behavior of the predicted CO:

- High values for the CO emissions are obtained due to the nature of diffusion flames and the high temperatures reached in oxy-fuel combustion, as it has been posed before.
- The trends predicted for the CO seem to be collapsed when comparing the different fuel mixtures at lean conditions. However, the results obtained for the stoichiometric point differ significantly of the expected trend observed in the equilibrium calculations. Furthermore, Figures 60, 61 and 62 clearly show that mixtures with higher content of heavier hydrocarbons produce less CO than mixtures with larger amount of CH₄, at the stoichiometric point.
- The values for the CO are again triggered at the stoichiometric point. Since CO is generally produced by the incomplete reaction of carbon containing fuels, and the excess of oxygen helps to complete the fuel combustion. Therefore the produced CO is decreased at equivalence ratios below the stoichiometric one [2].

6 Conclusions

The functionality of the Oxy-Fuel Burner as a low emissions technology has been evaluated in this project, also different case scenarios, such as the consequences of operating at lean conditions or the effect of changing the fuel composition, have been analyzed. The following points aim to serve as brief summary of the results obtained for the studied cases and the methodology:

- The approach consisting on carrying out first the CFD simulation, then extract the equivalent reactor network (CRN) and solve it with a detailed chemistry set, has proved to generally provide reasonable values for the emissions. Those trends are in good agreement with the first approximation obtained with the equilibrium calculation, which is considered as an upper limit for the obtained values due to the assumptions of the equilibrium state. However, further experimental data is found to be required to confirm the effectiveness of the model and the procedure.
• Higher temperatures, better heat transfer rates and less pollutant emissions serve to summarize the benefits of using oxygen instead of air. In addition to that, the purity of the CO₂ concentration in the product gases is maximized, which eases its posterior capture.

• Hydrogen enriched mixtures and mixtures with heavier hydrocarbons have resulted in slightly higher flame temperatures, whereas the flame temperatures of the biogas mixtures are considerable lower than the temperatures of the 100% CH₄ case. Consequently, it can be conclude that type 1 and type 2 mixtures have no significant effect on the overall efficiency of the burner in terms of heat transferred, whilst the biogas mixtures have presented a decrease of it.

• When comparing the NOx concentration at the flue gases, the hydrogen enriched mixtures and the heavier hydrocarbon mixtures have yielded into a significant increase of it. However, if the comparison is based on a produced mass basis, the trends become more similar and tend to collapse on a single curve. Regarding the biogas mixtures, either the concentration based or the mass based comparison show that the NOx are reduced when increasing the CO₂ content of the mixture.

• The CO levels have been reduced with the hydrogen enriched and the biogas mixtures. When it comes to the mixtures with heavier hydrocarbon levels, no clear conclusions could have been extracted due to the opposed trends shown by the CFD+CRN and the equilibrium calculations, especially at the stoichiometric point. However, the rest of the studied points have yield very similar values between fuels, which match the expected behavior obtained with the equilibrium calculations.

• For all the fuel mixtures, operating at lean conditions (with excess of oxygen) leads to a scenario of higher NOx, mainly due to the fact that the poor temperature drop does not outweigh the increased amount of N₂ entering the chamber, which is a limiting reactant to the formation of NOx. Conversely, the CO emissions are reduced dramatically by just operating at slightly lean conditions due to the help provided by the excess of oxygen to complete the combustion of the carbon containing fuels. Thus, in order to optimize the burner performance, operating at equivalence ratios between 0.9 and 1 has proved to be the solution that better compromises the overall efficiency of the system while maintaining the pollutant emissions at reasonable levels.

• For interchangeable fuel mixtures, the trends for the oxyfuel burner indicate that with addition of hydrogen or higher hydrocarbons that NOx will increase, especially for hydrogen. Addition of CO₂ will reduce NOx. CO is reduced by addition of hydrogen but is increased with addition of higher hydrocarbons and CO₂.
Appendix A: Details of the domain modeled

Domain dimensions

Figure A-1 contains the dimensions of the domain modeled, which have been extracted from the product information available at the Eclipse website [8]. All the values are given in millimeters.

Boundary conditions

The different boundary conditions that have been modeled are highlighted in Figure A-2 to Figure A-12.
Figure A-2: Brick walls.

Figure A-3: Chimney wall.
Figure A-4: Fluid domain.

Figure A-5: Fuel inlet.
Figure A-6: Fuel walls.

Figure A-7: inner oxygen walls.
Figure A-8: outer oxygen walls.

Figure A-9: outlet.
**Figure A-10:** oxygen inlet.

**Figure A-11:** pre-combustor walls.
It represents the named selection of all the blocks of the domain. A material for this zone needs to be specified, and the pdf-mixture created by the Partially Premixed model has been therefore selected. As it has been presented before, radiation has a significant role in the heat transfer scenario, and here lies the importance of selecting the proper way to compute the absorption coefficient of the material. The default Weighted Sum of Grey Gases Model (WSGGM-domain based) has been selected, since there is no significant difference between it and a special WSGGM for oxy-fuel atmospheres when the beam length ($S$) of the domain, given by Equation 1, is below 10 m, as discussed by [16].

$$S = 3.6 \cdot \frac{V}{A}$$

*Equation 4: Beam length expression.*

Where $V$ is the volume of the domain and $A$ is the surface area of the domain. Assuming that the domain is composed only by the furnace and that it is a rectangular prism, the previous equation yields to a beam length of 0.7 m, being then the default WSGGM valid for the current application.

**Fuel inlet**

Once the fuel composition and the required thermal power are given, the fuel mass flow rate is computed by dividing the thermal power by the low heating value of fuel mixture (LHV) [2]. Information about the turbulence at the inlet is provided by the hydraulic diameter and the turbulent intensity. The formulas used to calculate both parameters are presented in Equations 2 and 3, respectively.
\[ D_h = 4 \cdot \frac{A}{P} \]

Equation 5: Hydraulic diameter formula.

Where \( A \) is the cross sectional area and \( P \) is the wetted perimeter of the cross section.

\[ I_{turb}(\%) = \frac{0.16}{Re_{D_h}^{\frac{1}{8}}} \]

Equation 6: Inlet turbulent intensity formula [14].

This formula is employed under the assumption of fully developed duct fluid flow at the inlet [14]. \( Re_{D_h} \) is the Reynolds number for the hydraulic diameter at the inlet, which it is an input since the fuel composition and the mass flow rate are inputs, being then the velocity of the flow, the density and the viscosity known variables. The inlet temperature and pressure are assumed to be 300 K and 1 atm, respectively.

Finally, the mean mixture fraction is fixed to 1 for the boundary conditions needed by the species model, as it corresponds to the fuel inlet when working with the Partially Premixed model.

**Oxidizer inlet**

In order to obtain the oxidizer mass flow rate the following variables are required: the desired equivalence ratio (\( \Phi \)), which follows the expression of Equation 4, and subsequently, the fuel mass flow rate.

\[ \Phi = s \cdot \frac{\dot{m}_{fuel}}{\dot{m}_{oxidizer}} \]

Equation 7: Expression for the equivalence ratio [17].

Where \( \dot{m}_{fuel} \) and \( \dot{m}_{oxidizer} \) are the fuel and oxidizer flow rates, respectively. The \( s \) variable corresponds to the mass stoichiometric ratio, which is computed using the expression of Equation 5.

\[ s = \frac{v'_O \cdot MW_O}{v'_F \cdot MW_F} \]

Equation 8: Mass stoichiometric ratio [17].

\( MW_O \) and \( MW_F \) are the molecular weights of the oxidizer and fuel mixtures respectively, which can be directly calculated since both compositions are known. \( v'_O \) and \( v'_F \) correspond to the stoichiometric coefficients when considering an overall unique reaction of the type:

\[ v'_F \cdot Fuel + v'_O \cdot Oxidizer \rightarrow Products \]

Equation 9: General combustion reaction.

The parameters regarding the turbulence information are obtained by following the same procedure used for the fuel inlet. The inlet temperature and pressure are assumed to be 300 K and 1 atm, respectively. Finally, no change is needed for the boundary conditions related to the species model since the default value of 0 for the species variables matches the theoretical conditions at the oxidizer inlet.
Outlet

The outlet of the furnace remains at the atmospheric pressure, which is in agreement with the default value of 0 Pascal for the gauge pressure. Table A-1 presents the information of the turbulence and other parameters that have been employed for the pressure outlet boundary condition.

<table>
<thead>
<tr>
<th>Variable [units]</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Gauge pressure [Pa]</td>
<td>0</td>
</tr>
<tr>
<td>Backflow turbulent kinetic energy ([m^2/s^2])</td>
<td>1</td>
</tr>
<tr>
<td>Backflow turbulent dissipation rate ([m^2/s^3])</td>
<td>1</td>
</tr>
<tr>
<td>Backflow temperature [K]</td>
<td>1500</td>
</tr>
<tr>
<td>Backflow progress variable</td>
<td>1</td>
</tr>
</tbody>
</table>

The default values for the backflow turbulent kinetic energy and turbulent dissipation rate are used, as these values have also been employed in other studies [16]. The backflow temperature is set to 1500 K as a rough estimation of the outlet temperature. Finally, the backflow progress variable is set to 1 in order to indicate that at the outlet the reaction is completed.

Chimney wall

The default properties of this wall have not been modified, being therefore an adiabatic wall.

Brick walls

The brick walls represent the furnace walls, which are usually water cooled during experimental runs, in order to simulate the load that is present while operating under normal conditions. Thus convection option has been selected for these walls, but also due to the benefits (in terms of the stability of the numerical simulation) that presents when compared with the fixed temperature or fixed heat transfer rate options. Table A-2 gathers the material and thermal properties that are required.

<table>
<thead>
<tr>
<th>Material name</th>
<th>Brick</th>
</tr>
</thead>
<tbody>
<tr>
<td>Conductivity ([W/m\cdot K])</td>
<td>4</td>
</tr>
<tr>
<td>Thickness [mm]</td>
<td>150</td>
</tr>
<tr>
<td>Heat transfer coefficient ([W/m^2\cdot K])</td>
<td>250</td>
</tr>
<tr>
<td>Free stream temperature [K]</td>
<td>298</td>
</tr>
<tr>
<td>Internal emissivity</td>
<td>0.6</td>
</tr>
</tbody>
</table>

With this set of parameters the solution reached when modelling pure methane combustion yields a wall temperature at around 1800 K, well below the melting point of the ceramic materials usually employed in industrial furnaces, and also a heat flux of approximately 35 kW/m². These results are in agreement with the experimental data extracted from [19].
Pre-combustor walls

As its name denotes, the pre-combustor walls represent the delimitating walls of the pre-combustor chamber, which are made of an insulating material in order to prevent high temperatures at the burner nozzle that compromise its proper functioning. Instead of using the adiabatic wall option, the convection one has been preferred. Table A-3 summarizes the properties of the material for this wall and the convective properties, which pretend to model the insulating capacity exposed before.

<table>
<thead>
<tr>
<th>Boundary name</th>
<th>Brick 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Conductivity [W/m·K]</td>
<td>0.32</td>
</tr>
<tr>
<td>Thickness [mm]</td>
<td>200</td>
</tr>
<tr>
<td>Heat transfer coefficient [W/m²·K]</td>
<td>250</td>
</tr>
<tr>
<td>Free stream temperature [K]</td>
<td>298</td>
</tr>
<tr>
<td>Internal emissivity</td>
<td>0.75</td>
</tr>
</tbody>
</table>

As it can be noticed, the thermal resistance derived from the pre-combustor wall properties is much higher than the associated with the brick walls, being then the heat lost through the pre-combustor negligible.

Fuel and inner oxygen walls

They both represent the surface of the solid part inside the burner nozzle whose function is to maintain separated the oxygen and fuel streams. The heat lost through one of this walls is gained by the other one, as it can be demonstrated with a simple heat balance. Also, this amount of transferred heat can be considered negligible, since the both streams are at the same temperature when flowing through the burner nozzle. Taking into account these points, it has seem reasonable to leave the adiabatic condition for these walls.

Outer oxygen walls

The outer oxygen walls represent the outer walls of the burner nozzle, which surround the oxygen stream. The convection option has been also chosen for this boundary condition, whose properties are shown in Table A-4.

<table>
<thead>
<tr>
<th>Material name</th>
<th>Steel</th>
</tr>
</thead>
<tbody>
<tr>
<td>Conductivity [W/m·K]</td>
<td>16.27</td>
</tr>
<tr>
<td>Thickness [mm]</td>
<td>4</td>
</tr>
<tr>
<td>Heat transfer coefficient [W/m²·K]</td>
<td>250</td>
</tr>
<tr>
<td>Free stream temperature [K]</td>
<td>298</td>
</tr>
<tr>
<td>Internal emissivity</td>
<td>0.85</td>
</tr>
</tbody>
</table>
Even though the properties presented in Table A-4 would yield to a low thermal resistance, the insulating role of the pre-combustor appears, and the solution shows that the heat lost through these outer walls is practically negligible.

**Symmetric planes**

No modifications on the defaults settings have been done since they are not needed for this type of boundary condition.
Appendix B: Reactor network sensitivity analysis

The gathered results of the sensitivity analysis are shown in Figure B-1 to Figure B-24. The analysis has been done on the stoichiometric case for each of the mixtures of each type.

Fuel type 1: Hydrogen mixtures

80% CH₄-20% H₂

Figure B-1: NO mass fraction vs. Number of reactors for 80% CH₄-20% H₂.

Figure B-2: CO mass fraction vs. Number of reactors for 80% CH₄-20% H₂.
50% CH₄-50% H₂

Figure B-3: NO mass fraction vs. Number of reactors for 50% CH₄-50% H₂.

Figure B-4: CO mass fraction vs. Number of reactors for 50% CH₄-50% H₂.
40% CH₄-60% H₂

Figure B-5: NO mass fraction vs. Number of reactors for 40% CH₄-60% H₂.

Figure B-6: CO mass fraction vs. Number of reactors for 40% CH₄-60% H₂.
30% CH₄-70% H₂

Figure B-7: NO mass fraction vs. Number of reactors for 30% CH₄-40% H₂.

Figure B-8: CO mass fraction vs. Number of reactors for 30% CH₄-70% H₂.
Fuel type 2: Landfill/digester biogas
96% CH₄-4% O₂

Figure B-9: NO mass fraction vs. Number of reactors for 96% CH₄-4% CO₂.

Figure B-10: CO mass fraction vs. Number of reactors for 96% CH₄-4% CO₂.
60% CH₄-40% O₂

**Figure B-11**: NO mass fraction vs. Number of reactors for 60% CH₄-40% CO₂.

**Figure B-12**: CO mass fraction vs. Number of reactors for 60% CH₄-40% CO₂.
55% CH₄-45% O₂

**Figure B-13:** NO mass fraction vs. Number of reactors for 55% CH₄-45% CO₂.

**Figure B-14:** CO mass fraction vs. Number of reactors for 55% CH₄-45% CO₂.
45% CH₄-60% O₂

**Figure B-15:** NO mass fraction vs. Number of reactors for 45% CH₄-55% CO₂.

**Figure B-16:** CO mass fraction vs. Number of reactors for 45% CH₄-55% CO₂.
Fuel type 3: Mixtures with heavier hydrocarbons

85% CH₄-15% C₂H₆

Figure B-17: NO mass fraction vs. Number of reactors for 85% CH₄-15% C₂H₆.

Figure B-18: CO mass fraction vs. Number of reactors for 85% CH₄-15% C₂H₆.
75% CH₄-25% C₂H₆

Figure B-19: NO mass fraction vs. Number of reactors for 75% CH₄-25% C₂H₆.

Figure B-20: CO mass fraction vs. Number of reactors for 75% CH₄-25% C₂H₆.
Figure B-21: NO mass fraction vs. Number of reactors for 75% CH₄-25% C₃H₈.

Figure B-22: CO mass fraction vs. Number of reactors for 75% CH₄-25% C₃H₈.

75% CH₄-25% C₃H₈
$75\% \text{CH}_4-15\% \text{C}_2\text{H}_6-10\% \text{C}_3\text{H}_8$

Figure B-23: NO mass fraction vs. Number of reactors for 75% CH$_4$-15% C$_2$H$_6$-10% C$_3$H$_8$.

Figure B-24: CO mass fraction vs. Number of reactors for 75% CH$_4$-15% C$_2$H$_6$-10% C$_3$H$_8$. 
Appendix C: Equilibrium calculations

The equilibrium model available in the CHEMKIN PRO software has been employed to perform all the simulations that follow this section [25].

N\textsubscript{2} effect

Figure C-1 to Figure C-3 show how the amount of nitrogen that the oxidizer stream contains affects the temperature, NO and CO concentrations, respectively, assuming that the equilibrium is reached.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{temperature_vs_equivalence_ratio.png}
\caption{Equilibrium temperature [K] vs. equivalence ratio for the different oxidizer mixtures.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{no_vs_equivalence_ratio.png}
\caption{Equilibrium NO [mass fraction] vs. equivalence ratio for the different oxidizer mixtures.}
\end{figure}
Figure C-3: Equilibrium CO [mass fraction] vs. equivalence ratio for the different oxidizer mixtures.

**Fuel type 1: Hydrogen mixtures**

Figure C-4 to Figure C-6 present the results obtained for the temperature, NO and CO mass fractions, assuming the equilibrium is reached, for the type 1 fuel mixtures.

Figure C-4: Equilibrium temperature [K] vs. equivalence ratio for the different type 1 mixtures.
Figure C-5: Equilibrium NO [mass fraction] vs. equivalence ratio for the different type 1 mixtures.

Figure C-6: Equilibrium CO [mass fraction] vs. equivalence ratio for the different type 1 mixtures.

Fuel type 2: Landfill/digester biogas

In Figure C-7 to Figure C-9 the temperature and the NO and CO mass fractions, respectively, can be found for the different mixtures of the type 2, assuming the equilibrium is reached.
Figure C-7: Equilibrium temperature [K] vs. equivalence ratio for the different type 2 mixtures.

Figure C-8: Equilibrium NO [mass fraction] vs. equivalence ratio for the different type 2 mixtures.
Fuel type 3: Mixtures with heavier hydrocarbons

The temperatures and the NO and CO mass fractions obtained for the different type 3 mixtures, with the equilibrium assumption, are presented in Figure C-10 to Figure C-12.
Figure C-11: Equilibrium NO [mass fraction] vs. equivalence ratio for the different type 3 mixtures.

Figure C-12: Equilibrium CO [mass fraction] vs. equivalence ratio for the different type 3 mixtures.

References

[1] “Fossil fuel energy consumption (% of total).”.


[18] “Engineering ToolBox.”.


[20] and Z. Q. Gregory P. Smith, David M. Golden, Michael Frenklach, Nigel W. Moriarty, Boris Eiteneer, Mikhail Goldenberg, C. Thomas Bowman, Ronald K. Hanson, Soonho Song, William C. Gardiner, Jr., Vitali V. Lissianski, “GRI 3.0 mechanism.”.


