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OXYGEN-ENRICHED COMBUSTION IN A GLASS MELTING FURNACE

A CFD STUDY

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Abstract

The goal of the Paris Agreement Conference in 2015 was to discuss the reduction of greenhouse gas emissions and limit global temperature rise. Energy-intensive industries, including the glass industry, face challenges such as high costs and emissions. The high costs associated with emissions emphasize the need for emission reduction measures. Oxygen enrichment in combustion is an energy-saving technology used in various high-temperature environments, but its application is limited due to production costs and retrofitting requirements of industrial equipment.

This work focuses on the modeling through computational fluid dynamics of oxy-natural-gas combustion in an end port regenerative furnace with a nominal capacity of 410 t_{glass}/day. In this project, ANSYS software was used to simulate the combustion chamber considering unsteady state, the realizable k- ϵ model for turbulence modeling, the discrete ordinate method and non-premixed natural gas-air combustion. The simulations use 21%, 25%, 30%, 35% and 40% of oxygen in the inlet while reducing the nitrogen flow rate. The simulations allow to analyze the energy availability, flame interaction, temperature and velocity fields and NO_x, CO and CO₂ concentration at the outflow stream.

As the combustion air was enriched with O₂ at the inlet, the heat available for glass melting showed a slight increase between 14808 kW and 15179 kW, with more heat released for glass melting due to the reduced N₂ flow rate. The main quantitative and qualitative results show that the maximum temperature in the combustion chamber increases with higher oxygen concentrations, ranging between 2399°C and 2516°C, which provides an improved combustion efficiency. Generally, the flame length is also affected by oxygen enrichment showing a shorter flame at higher O₂ concentrations. Flue gas temperature exhibits a slight rise between 21% and 40% of oxygen concentrations, from 1266°C to 1335°C.

The study also examines the mass fractions of CO, CO₂ and NO_x in the flue gas. The first decreases from 3.17×10^{-3} to 8.05×10^{-3} when enriching the inlet stream with O₂. The second presents mass fractions between 0.099 and 0.198, showing an upward behavior and indicating closer approximation to complete combustion. The concentration of NO_x increases gradually from 3.97×10^{-3} to 5.75×10^{-3} as O₂ inlet concentration increased from 21% to 40% due to the higher temperatures which promote the formation of thermal-NO_x.

Keywords:

Oxygen, Greenhouse emissions, Computational Fluid Dynamics, transient behavior, non-premixed combustion

Resumo

O objetivo da Conferência do Acordo de Paris em 2015 consistiu em reduzir as emissões de gases de efeito de estufa e limitar o aumento da temperatura global. As indústrias de utilização intensiva de energia, incluindo a indústria vidreira, enfrentam desafios como os custos elevados e as suas emissões. Assim, o enriquecimento de oxigénio na combustão surge como uma tecnologia de poupança de energia em vários ambientes de alta temperatura. No entanto, a sua aplicação é limitada devido aos custos de produção e aos requisitos de adaptação das instalações industriais.

Neste trabalho utiliza-se a modelagem de uma combustão oxi-gás natural num forno regenerativo com capacidade nominal de 410 toneladas de vidro por dia, usando a dinâmica de fluidos computacional. Neste projeto, o software ANSYS foi utilizado para simular a câmara de combustão estudada. Considerou-se estado não estacionário, o modelo $k-\epsilon$ para a turbulência, e a combustão turbulenta não pré-misturada do gás natural-ar. Analisou-se concentrações de 21%, 25%, 30%, 35% e 40% de O_2 na entrada e um caudal de azoto reduzido à medida que a composição de O_2 aumentava, com vista a prever a energia disponível, a interação da chama, os campos de temperatura, a magnitude das velocidades e a formação de NO_x , CO e CO_2 na saída.

À medida que o ar de combustão foi enriquecido com O_2 na entrada, o calor disponível para a fusão do vidro apresentou valores ligeiramente crescentes entre 14808 kW e 15179 kW, havendo mais calor libertado para a fusão do vidro devido à redução do caudal de N_2 . Os principais resultados quantitativos e qualitativos mostram que a temperatura máxima na câmara de combustão aumenta para concentrações de oxigénio mais elevadas, variando entre 2399°C e 2516°C, o que proporciona uma melhor eficiência na combustão. De um modo geral, o comprimento da chama também é afetado, apresentando uma chama mais curta a concentrações mais elevadas de O_2 . As temperaturas dos gases de combustão apresentam um ligeiro aumento entre 1266°C e 1335°C, à medida que a concentração de O_2 também aumenta.

Este estudo analisa também as frações mássicas de CO, CO_2 e de NO_x nos gases de combustão. O primeiro varia entre 3.17×10^{-3} e 8.05×10^{-3} quando se enriquece a corrente de entrada com O_2 , mostrando um comportamento decrescente. O segundo apresenta frações mássicas entre 0,099 e 0,198, mostrando um comportamento ascendente e indicando uma maior aproximação à combustão completa. O terceiro aumenta gradualmente entre 3.97×10^{-3} e 5.75×10^{-3} à medida que a concentração de O_2 na entrada aumenta de 21% para 40%, devido às temperaturas mais elevadas que promovem a formação de NO_x térmico.

Palavras-chave: Oxigénio, Emissões de Gases de Efeito de Estufa, dinâmica de fluidos computacional, estado transiente, combustão não pré-misturada

Declaration

I hereby declare, under word of honour, that this work is original and that all non-original contributions are indicated and due reference is given to the author and source.

A handwritten signature in dark ink, reading "Inês Marante Mesquita". The signature is written in a cursive style with a horizontal line underneath it.

(Inês Marante Mesquita)

Porto, 27th of July 2023

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Notation and Glossary

c_p	specific heat	J/(kg.K)
D_m	diffusion coefficient	m ² /s
f	mixture fraction	
h	enthalpy	J
	heat transfer coefficient	W/(m ² .K)
I	radiative intensity	W/m ²
J	diffusion flux	kg/(m ² .s)
k	turbulent kinetic energy	m ² /s ²
n	refractive index	
P	pressure	Pa
R	net generation rate	kg/s
S_{c_t}	turbulent Schmidt number	
S_T	heat source term	
T	temperature	K
u	velocity vector	m/s
Y	mass fraction	
x	position vector	
Z_k	mass fraction of species k	

Greek Letters

α	absorption coefficient	
α_λ	spectral absorption coefficient	
β	extinction coefficient	
δ	Kronecker delta	
ε	rate of dissipation	m ² /s ³
λ	wavelength	m
μ_t	turbulent viscosity	kg/m.s
ρ	density	kg/m ³
σ_s	scattering coefficient	Pa
τ	viscous stress tensor	
φ	scattering phase function	
ϕ	Favre-averaged values	
Ω	solid angle	

Indexes

i, j, l	index or counter
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List of Acronyms

AO	Air-Oxygen-Fuel Combustion
BECCS	Bioenergy with Carbon Capture and Storage
BEIS	Business, Energy, and Industrial Strategy
CC	Combustion Chamber
CCU/CCS	Carbon Capture, Utilization, and Storage

CFD	Computational Fluid Dynamics
DOM	Discrete Ordinate Method
EII	Energy-Intensive Industries
EU ETS	European Union Emissions Trading System
GHG	Greenhouse Gas
HRS	Heat Recovery System
IS	Individual Sections
ORC	Organic Rankine Cycle
PDF	Probability Density Function
PE	Premix Enrichment
REN	Redes Energéticas Nacionais
RTE	Radiative Transfer Equation

1 Introduction

1.1 Framing and Presentation of the Work

To achieve the desired reduction in Greenhouse Gas (GHG) emissions, the Paris Agreement Conference in 2015 implemented goals to decarbonize the energy, residential, commercial, and industrial sectors. The Agreement established to limit global temperature from rising to well below 2°C above pre-industrial levels, and pursue efforts to limit the temperature increase to 1.5°C. To reach these goals, it is necessary to face some challenges that Energy-Intensive Industries (EII) involve, such as their high capital and production costs, competitiveness needs, and quality standards. The amount of energy used per ton of product characterizes the EII and, for instance, the glass energy consumption corresponds to a range from 4 to 17 GJ/t, depending on the glass sub-sector (container glass, flat glass, special glass, or glass fibers).

Over the years, the amount of carbon dioxide (CO₂) released in container and flat glass sector has decreased significantly, and in Europe, 60 Mt of CO₂ were emitted in 2007, 18 Mt of CO₂ in 2019 and 3.2 Mt of CO₂ in 2019. Most of the energy needed in glass manufacturing goes to the high temperatures required to melt the raw materials. The container and flat glass industry releases 47% and 33% of the total glass manufacturing emissions, respectively (Rio et al., 2022; Zier et al., 2021).

1.1.1 CO₂ Pricing

CO₂ pricing is a policy approach created to incentivize the mitigation of GHG emissions with two types of systems: carbon taxes and cap-and-trade. The first one consists in direct taxes on the carbon content of fossil fuels or on the emissions of CO₂ that result from their combustion, while the second establishes a limit on the total amount of CO₂ that can be released in a certain time, and then allocate emissions allowances to businesses or other entities. A market is set up based on the individual emissions levels and needs of entities, being able to buy or sell these allowances among themselves (Zier et al., 2021).

Comparing the CO₂ emissions between China and Europe shows that the first one presents bigger values, around 0.49 tCO₂/t_{glass}, and the second one about 0.46 tCO₂/t_{glass}. The fuel mix explains the disparity in values because while in China fossil fuels are mainly used (coal, natural gas, and oil), in Europe, natural gas accounts for about 90% of the energy consumed by the glass manufacturing industry (Hu et al., 2018; Zier et al., 2021).

Figure 1 illustrates that the CO₂ market faced some changes and developments over the years since 2008. In 2005, the European Union Emissions Trading System (EU ETS) was launched as the first and largest emissions trading system. As Zier et al. (2021) mentioned, at the beginning,

the prices of carbon even surpassed 30 €/tCO₂ followed by a crash to below 10 €/tCO₂ until 2018. In the 2020s, CO₂ market continued to grow, and the prices increased globally. The EU ETS expects an increase of the CO₂ price with the selection of new technologies or fuel switch (Zier et al., 2021).



Figure 1 - Time series of EU emission Allowance (EUA) price (Zier et al., 2021).

For instance, in April of 2021, a Portuguese container glass industry producing 470 tons of glass per day, and considering an emission of 0.46 tCO₂/t_{glass}, over a year will spend around 3.3M€, showing why it is crucial to develop new measures to reduce the emissions that contribute environmental and economically.

1.1.2 Oxygen Enrichment in Combustion

In the present section, the combustion process in the combustion chamber (CC) will be briefly discussed considering the amount of flue gas released and the energy consumption.

Oxygen combustion technology is one of the useful energy-saving technologies for combustion systems. In conventional air/fuel combustion, nitrogen acts as an inert gas and absorbs some of the energy to form the flue gas, which contributes to a reduction of the fuel utilization efficiency. In contrast, oxygen combustion technology decreases the amount of nitrogen involved in the reaction. The benefits allowed by this technology include higher thermal efficiency, lower thermal energy loss through flue gases, higher available heat, higher reduction rate, etc. Oxygen combustion is widely used in high temperature environments such as aluminum remelting furnaces, incinerators, glass melting furnaces and ladle furnaces. However, the cost to produce oxygen is high, which limits the utilization of this technology in several equipment. Moreover, to apply oxy-fuel systems, the burner and furnace body would

have to be modified to avoid problems related with heat transfer, flame structure and damage to refractories, which would not be feasible as the cost of retrofitting would be very high. Changing the oxygen concentration while applying oxygen enriched combustion to current traditional air/fuel burners may be the answer (Baskar & Senthilkumar, 2016; Wu et al., 2010).

Bisio et al. (2002) indicated that various investigations have shown a considerable reduction in unburned hydrocarbons, carbon monoxide (CO) emissions and smoke, while nitrogen oxide (NO_x) emissions increase proportionally with the increase of oxygen concentration due to the increase in flame temperature. Numerous aspects, including the design of the combustion system, the operating conditions, and the application of the proper controls and technologies, must be considered to properly manage and decrease NO_x emissions.

The purpose of this study is to investigate the effects of oxygen enriched combustion in an end port regenerative furnace with different levels of O₂ concentration through Computational Fluid Dynamics (CFD).

1.2 Presentation of the Company

One of the largest manufacturers of glass containers for the food and beverage sector in Europe is BA Glass B.V. The history of the company began in 1912 with the incorporation of the company 'Barbosa e Almeida', producing and commercializing only bottles by partners Raúl da Silva and Domingues de Almeida. In 1930, a new technology (semi-automatic) was introduced to launch industrial activity and the name was changed to 'Fábrica de Vidros Barbosa e Almeida, Lda.'. With the installation of an automatic feeding mechanism and a molding machine in 1947, the automated technology allowed a significant development of the company.

A few years later, in 1965, the company sought higher production and purchased a third automatic machine that could produce 350 thousand bottles per week. At the end of the 1960s, a new industrial plant was put into operation in Avintes, consisting of two regenerative furnaces (with heat recovery). In 1975, the business had established itself as a limited liability company under the name 'BA - Fábrica de Vidros Barbosa & Almeida, SARL' and installed numerous IS machines, including a computerized one.

In the late 1980s, José Augusto da Silva Domingues acquired shares in Sogrape (77%), and Vinícola Vale do Dão (3%), owning 80% of the company's capital. To increase the production of glass packaging in Portugal, a new furnace was built, which allowed an expansion of about 40%. In 1993, 'CIVE - Companhia Industrial Vidreira, SA', located in Marinha Grande and owned by the Portuguese State, was acquired by BA with a capacity of three melting furnaces. The merger between CIVE and BA took place in 1995, and the Sonae Group acquired a substantial stake in BA Glass in 1998. In the following years, the Spanish company 'BA - Fabrica de Envases de Vidrio

Barbosa & Almeida, SA' was integrated and a single furnace plant was built in Villafranca de los Barros. Sonae Group's ownership grew, and BA Glass proceeded to expand its market position by acquiring companies such as Sotancro Group and Anchor Glass.

In 2016, BA acquired a glass packaging company in Germany, which allowed it to expand its market in Central Europe. The company's expansion continued in 2017 with the acquisition of four plants in Athens, Sofia, Plovdiv, and Bucharest. This expansion enabled production of more than 20 million units per day. Recently, BA has taken a significant step forward in its international expansion, acquiring a majority shareholding in a relevant Mexican Glass Packaging producer 'Vidrio Formas' (Homepage - BA Glass, 2023).

1.3 Contribution of the Author to the Work

First and foremost, getting to know the company and the Batch and Furnace Department was essential to understand the specifics of each variable involved in the combustion process. To carry out this work, it was necessary to become thoroughly familiar with the ANSYS software, which meant spending a considerable amount of time at this initial stage. Also, understanding the combustion requirements in the combustion chamber under study was an important part of this dissertation, since it allowed to model the process for the CFD simulations. The post processing results (quantitative and qualitative) was the last part analyzed and discussed.

1.4 Organization of the Dissertation

This dissertation is divided into 5 chapters. The first chapter briefly introduces the topic of the internship and gives an overview of the history of the company.

Chapter 2 provides an overview of the *Best Available Technologies* in the glass industry, an introduction to glass production, a description of ANSYS's background and equations used in the models.

Chapter 3 frames the technical analysis of the main features of the studied combustion chamber.

Chapter 4 contains the simulation results, focusing on the energy consumption, velocity and temperature fields, and composition of the flue gas emissions.

Chapter 5 summarizes the results of the numerical simulations highlighting the main findings of this study and the comparison with other studies.

2 Context and State of the Art

To understand the objective of this dissertation, it is important to give a contextualization of the main challenge of the glass industry. Glass manufacturing is one of the energy-intensive industries due to the energy consumption per ton of product, the main consumer being the combustion reaction in the melting furnace, which also leads to a significant release of flue gas emissions. The production of glass is associated with direct and indirect emissions in several sectors. The first are from the combustion of fossil fuels and the degradation of raw materials in the furnace, while the second are generated by electricity from the power grid. The main primary gases released are CO_2 , NO_x and SO_x . According to Sardeshpande et al. (2007) , 22% of the energy introduced into the furnace corresponds to heat losses from flue gases, as shown in the Sankey diagram in Figure 2. Also, Rio et al. (2022) state that the production of 1 kg of glass in a gas-fired furnace produces about 0.6 kg of CO_2 (of which 0.45 kg is from fossil fuels) and 0.15 kg from the dissociation of carbonates. In Europe and the U.S., natural gas is the main fuel used (75-85%), followed by electricity (10-15%) and fossil fuels (5-10%), while in China, coal was the principal fuel consumed until 2010, indicating that there is an urgent need to reduce energy intensity in glass production. The solution to this challenge lies in electrification and the installation of hybrid technologies, switching from electricity to gas based on the price, which can reduce the amount of emissions by 78% (Rio et al., 2022). These technologies will be explored in more detail in the next subsection.

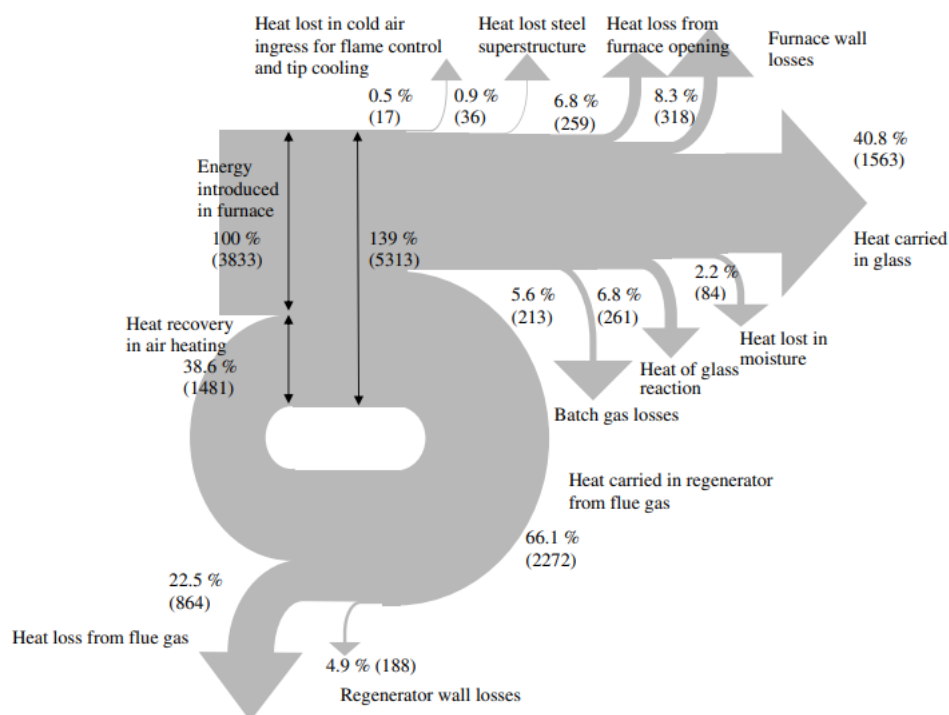


Figure 2 - Sankey diagram for a glass furnace (Sardeshpande et al., 2007).

2.1 Glass Manufacture

Glass production involves various processes, starting with the raw materials mixed in batch preparation, melting of the glass in the furnace, forming, post-forming, and finishing. The glass product goes through several process steps with different temperature levels and energy requirements (Homepage - BA Glass, 2023; Zier et al., 2021). In this chapter, the glass processes are briefly described.

2.1.1 Glass Manufacture Processes

Glass Composition

The raw materials that glass industry uses are silicon dioxide (SiO_2), 70-72%, sodium oxide (Na_2O), 12-14%, calcium oxide (CaO), 9-11%, magnesium oxide (MgO), 0-3%, aluminum oxide (Al_2O_3), 1-2%, and potassium oxide (K_2O), 0-1%. Taking into account the glass type ordered by the client, these components will be measured and mixed in order to create the mass composition appropriated. Thus, the raw materials composition's that enters the furnace can be made up of treated waste glass, and ground glass waste from internal and/or external recycling (Homepage - BA Glass, 2023).

Raw Materials Fusion

In refractory furnaces, material melting takes place at temperatures between 1500 °C and 1600 °C. The liquefied glass moves by gravity along the large container and then passes through the "tuning" phase, in which it is necessary to ensure the temperature uniformity of the entire molten mass, as it is a prerequisite to produce a high-quality product. This procedure outlines the methods for melting the glass batch to obtain the glass quality required for molding, as well as the control of the main environmental components of this process (Homepage - BA Glass, 2023).

Glass Forming

This phase includes two steps of the forming process: In the first mold, called "pre-form", the glass is exposed to the mold, which is inside the machine. In the second stage, the bottle passes through the final mold, which is on the other side of the machine, where it gives the final shape (Homepage - BA Glass, 2023).

Annealing and Surface Treatment

In this phase, the glass is in contact with the walls of the mold, which have low temperatures. Since the outer layers of the pieces are much colder than the inner ones, this leads to internal stresses, and to avoid this, it is necessary to proceed in a slower and more controlled way. Annealing is a process for eliminating all stresses of a thermal nature, which is ensured by

raising the temperature of the products to a level that allows the stresses to be relieved, followed by a slower and controlled cooling (Homepage - BA Glass, 2023).

Inspection and Quality Control

The next step concerns the quality check control of the final product, in which the bottles enter automatic inspection machines that sort out defective pieces through various defect detection mechanisms. The types of defects that appear in the glass are bubbles, stones, knots, cords, cracks, scratches, inclusions, devitrification, wrapping and swirls or streaks (Homepage - BA Glass, 2023).

Packaging

At the end of the production line, the glass packages are grouped into pallets in multiple layers. These are covered with plastic film to allow a safer and easier transportation. Then, these packages are shrunk in a furnace, and the pallets are transported to the storage area. Depending on the customer's requirements, some of them can be forwarded for labeling (Homepage - BA Glass, 2023).

2.1.2 End Port Regenerative Furnace

In the glass industry, one of the most frequent regenerative furnaces is the end-port type. In this subsection, it is described in detail to understand its operation and conditions.

According to Homepage - BA Glass (2023), end-port regenerative furnaces are typically used to produce more than 230 tons of glass per day. This industrial furnace consists of two main structures, the combustion chamber, and the heat recovery system (HRS), as shown in Figure 3. The CC is a refractory furnace where raw materials enter and melt at high temperatures through the combustion process. The temperatures required for glass melting range from 1400 to 1600 °C, and the exhaust gases leaving the CC reach 1300-1600 °C. The heat recovery system, which in this case is called a regenerator, is used to improve the overall efficiency by reusing the exhaust gases. This system can have two or more regenerative towers located at the end of the CC fed with air and exhaust gases in cycles of 20/30 minutes (Cravero & De Domenico, 2019).

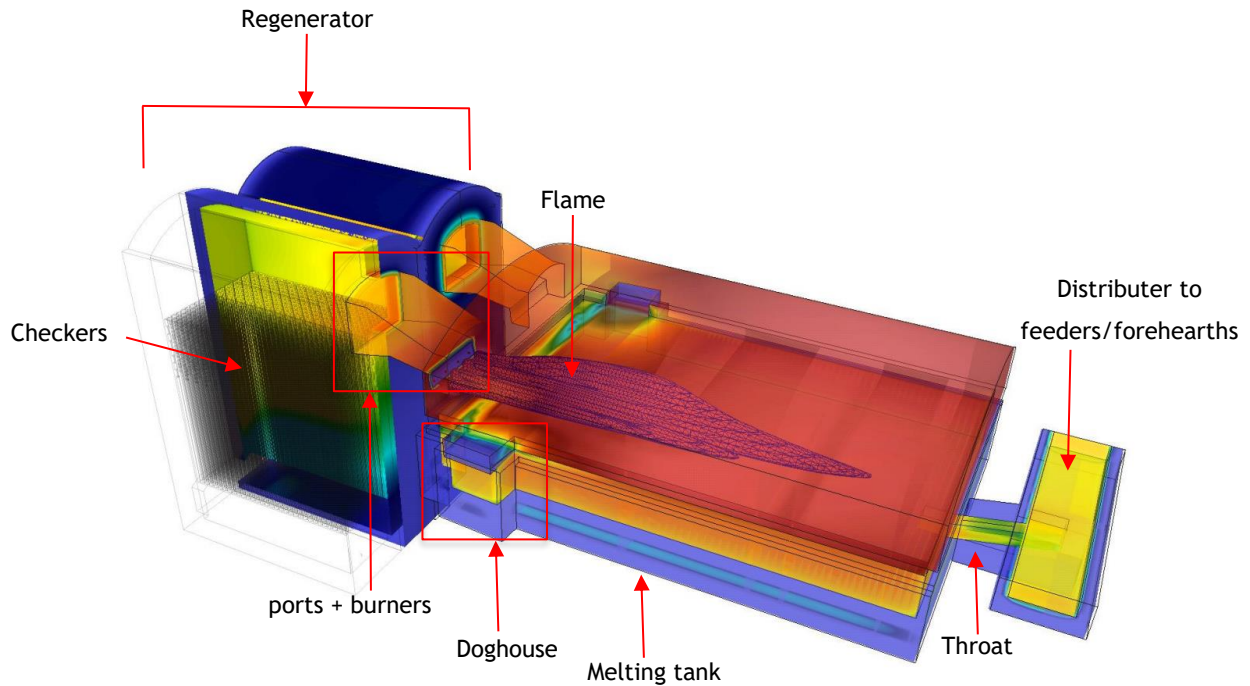


Figure 3 - End port regenerative furnace (edited screenshot) (Homepage - BA Glass, 2023).

The regenerator contains three zones of the regenerative chamber, namely the upper chamber, checkers zone and the lower chamber, where the compressed air is introduced and passes through the regenerator tower, being preheated by the recovery of waste heat from the exhaust gases, as already described. The air mixture arrives at the upper chamber and then enters at the ports. The fuel is usually introduced into the CC through burners, which creates the flame. The raw materials mixture in the doghouse feeds the furnace tank and subsequently, after obtaining the molten glass, this is fed into the throat, following to the forehearth (Ark hazloo et al., 2019).

2.1.3 Approaches and Technologies for Glass Decarbonization

Since the 19th century, the glass industry has sought to reduce energy demand. Despite efforts to transition to a low-carbon future, additional demand and supply-side interventions are required. Supply-side measures include retrofitting inefficient production facilities and deploying key technologies such as oxyfuel firing; batch and cullet preheating; carbon capture, utilization, and storage (CCU/CCS); electrification; biofuels; and hydrogen technologies. This section discusses technological innovations, practices, and legislation to decarbonize the glass industry, such as those previously mentioned. Collaboration between the public and private sectors is needed to develop innovative policy packages and voluntary measures to enable decarbonization. (Rio et al., 2022).

Carbon Capture, Utilization, and Storage

Some researchers state that the use of carbon capture and storage technologies is unavoidable due to the size and GHG dilution of conventional glass plants, while others view them as an additional strategy to mitigate GHG emissions. Adding a sequestration unit to the oxyfuel combustion process can reduce emissions by 75%. Thus, bioenergy with carbon capture and storage (BECCS) may be a better option than using fuels such as natural gas and hydrogen because their characteristics allow a more radiative flame, higher moisture content. However, there are still obstacles to overcome, such as high cost, low carbon trading prices, difficulties with capture technology, CO₂ transport, and storage locations. In addition, most of the glass producers are small units, making it difficult to invest in emission capture equipment (Griffin et al., 2021).

Batch Preheating

Previous studies showed that batch preheating is a mature and successful method for reducing emissions from the glass industry. This method can recover sensible heat and recapture dust and sulfur oxide (SO_x) by capturing hot exhaust gases and passing them through cullet or batch, resulting in significant energy savings, improved production rates, and lower CO₂ emissions. Batch preheating systems can be implemented in existing glass melting furnaces with cullet content greater than 50%, and some research indicate that excellent results can also be achieved with lower cullet content in the 30% to 40% range. The expected CAPEX and OPEX costs for a cross-fired regenerator glass melting furnace with a capacity of 350 tons per day are 1.5 M€ and 120 k€, respectively. Rio et al. (2022) also mentioned that the glass industry can reduce CO₂ emissions regionally by up to 1256 kt if this strategy is implemented throughout the European Union.

However, installation of batch preheating systems can be capital intensive and requires equipment of comparable capacity to the actual melting plant. In addition, if the cullet mixture exceeds the required amount, dust carryover and clogging problems can occur. Other developments, such as electric heating and insulation of the melter, require less waste heat for batch preheating (Rio et al., 2022).

Waste Heat Recovery

The glass industry research suggests that waste heat recovery is a viable alternative for reducing emissions. This method requires using the heat content of the furnace's exhaust gases, which generally accounts for 25-30% of the furnace's energy input. There are several types of waste heat recovery, including recovery of heat and electricity. The use of heat for thermal purposes, regulation of heat for external thermal applications, and generation of electricity with technologies such as Organic Rankine Cycle (ORC) are the most widely used techniques. In

this study, the CAPEX and OPEX expenses for this technology are estimated at 1.67 M€ and 33,500€ per year, respectively, for a 300 tons per day end-fired container glass furnace with heat extraction after an electrostatic precipitator (Hu et al., 2018).

Waste heat recovery has gained attractiveness in EII processes as it reduces industrial energy demand, increases energy efficiency, and improves air quality by reducing industrial pollutants and GHG emissions. Hu et al. (2018) demonstrated that installing a waste heat recovery power generation system on the glass line can result in significant energy savings and emission reductions, with the potential to save 28,500 tons of SO₂, 83 tons of NO_x, 33 tons of CO₂, and 79 tons of dust emissions. Several studies have shown that ORC could be a worthwhile investment for the glass sector if electricity costs are below the price of grid electricity. The technology has the potential to reduce the industry's environmental impact and contribute to a more sustainable future.

Biofuels

Although research on the use of biofuels to decarbonize the glass industry is sparse, some studies indicate that this is a promising way forward. When biofuels are paired with carbon capture technologies, glass manufacturing processes can generate net-negative CO₂ emissions. Some biofuels, such as biodiesel, are a good source of energy for glass manufacturing because their combustion generates high temperatures. However, they are more expensive, and can be a large contributor to the CO₂ footprint. Therefore, it is suggested that the use of biomass and waste as fuel must be considered when implementing policies and strategies. Biomethane is one of the biofuels that could be a potential candidate, as it absorbs CO₂ emitted during production, resulting in net zero emissions (Rio et al., 2022).

Many components of biomass ash can be used in commercial glass production to replace sand and limestone and minimize energy consumption and emissions. According to the Department for Business, Energy, and Industrial Strategy (BEIS), the UK has the biofuel capacity to supply the entire glass industry and can decarbonize existing glass furnaces at lower cost and with less infrastructure investment. The availability of biofuels, which the glass sector would need, is hindered by barriers such as cost, quality requirements, and supply difficulties (Rio et al., 2022).

Electrification

Some researchers propose that electric melting is the most energy efficient technology for furnaces. Nevertheless, commercial availability is still restricted to modest sizes, and it is not yet known if the technique can be scaled up to larger manufacturing processes (above 200 tons of daily production). For a container glass furnace with a capacity of 300 tons per day and heat

extraction after the electrostatic precipitator, the estimated investment cost for this method is about 1.67 M€ (Rio et al., 2022).

Electric furnaces are more efficient than conventional fossil fuel furnaces, resulting in lower energy losses and reduced NO_x emissions, as 35% of energy consumption is saved compared to conventional technology. Rio et al. (2022) demonstrated that converting the system to all-electric can be 31% more efficient than the usual technology and save about 5561 kT of CO₂ in the EU. Net carbon emissions can be more easily achieved if the power grid incorporates more low-carbon energy sources, which can reduce CO₂ emissions by up to 75%.

However, there are significant obstacles to the electrification of the glass sector, such as electricity demand that could increase by 170%, the high cost of electricity compared to alternative energy sources, and the incompatibility of electric melting with high-temperature glass furnaces with a daily output of more than 200 tons (Rio et al., 2022).

Hydrogen

Hydrogen has the potential to decarbonize numerous industrial sectors, including glass manufacturing. According to Griffin et al. (2021), the high temperature requirements of glass manufacturing favor the use of hydrogen and oxyfuel burners because they allow combustion with pure oxygen, reducing NO_x formation. However, compared to natural gas, hydrogen has technological disadvantages as it has a lower volumetric energy content and a less efficient flame. Therefore, further technological developments are needed to make hydrogen a viable fuel for glass production. Researchers are using computer simulations to investigate how the heating profile of hydrogen in glass furnaces can match that of natural gas.

Innovations in Heating and Melting

Oxy-fuel furnaces are a technology that uses oxygen enriched feed instead of air in the combustion reaction, which can reduce the amount of inert nitrogen transported or heated. This approach can result in a 60% to 70% reduction in flue gases compared to conventional combustion and reduce energy losses by 25-35% compared to a furnace without extra heat recovery. This technology has the advantage of saving about 5-20% of fuel, depending on the type of regenerator furnace. However, the implementation of this technology requires a comprehensive strategy, as the burner and the furnace body must be retrofitted and the use of pure oxygen is expensive (Rio et al., 2022; Zier et al., 2021).

Another possibility is the enrichment of oxygen in the combustion air feed, which leads to a lower energy requirement for the combustion of the combustible mixture and to a reduction in ignition delay and combustion noise. Baskar & Senthilkumar (2016) reported that by increasing the oxygen concentration, the combustion process can be completed faster and more efficiently, resulting in better fuel utilization and less waste. Another effect is an increase in

specific power output as more fuel is burned and more energy is released. Increased nitrogen oxides are one of the possible negative effects of oxygen enrichment.

To understand the influence of oxygen concentration on exhaust gas temperature, NO_x emissions and flame pattern including stability, shape and dimensions, a case study is presented in Bělohradský et al. (2014). The combustion test was conducted to investigate the effects of oxygen concentrations in the range of 21-46% by two oxygen-enriched combustion methods, namely premix enrichment (also referred to as PE) and air-oxygen-fuel combustion (referred to as AO). Figures 4, 5 and 6 show the results as a function of the oxygen content.

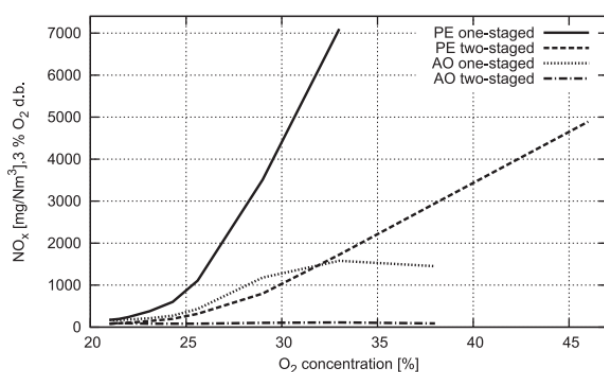


Figure 4 - Effects of oxygen concentration on the NO_x emissions (Bělohradský et al., 2014).

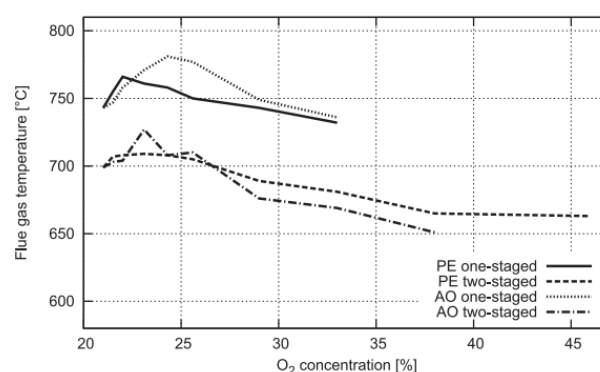


Figure 5 - Effects of oxygen concentration on the flue gas temperature (Bělohradský et al., 2014).

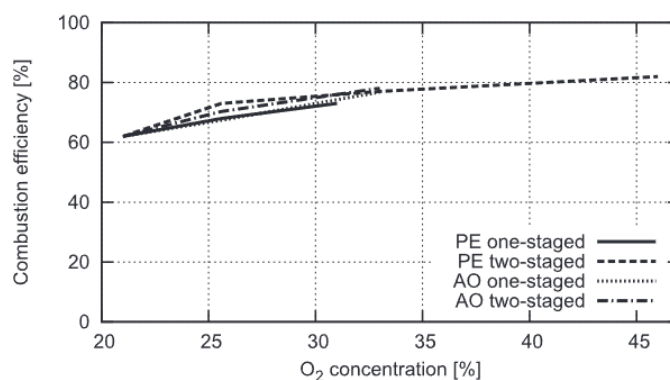


Figure 6 - Effects of oxygen concentration on the combustion efficiency (Bělohradský et al., 2014).

As can be seen in Figure 4, during PE tests, as the oxygen concentration is increased, the NO_x emission increases sharply due to a higher furnace temperature. From 21% to 33% in oxygen content, NO_x concentration increased more than 40-fold and 20-fold when single-stage and two-stage combustion units were used, respectively. In the experiments of AO, the emissions of NO_x were lower than in the first experiments. In AO two-staged tests, the concentration of NO_x released was always below 120 mg/Nm^3 . Figure 5 shows that the flue gas temperature increased

when oxygen content is 23-24%. Therefore, the higher the O_2 concentration, the lower the amount of N_2 and the lower the flue gas temperature. As shown in Figure 6, O_2 enrichment leads to an increase in combustion efficiency, which is less intense at higher concentrations.

2.2 Background of ANSYS Software

The ANSYS software or other solvers can be used for the analysis and optimization of furnace designs. The software can be used to improve furnace efficiency, increase product quality, reduce emissions, and extend furnace life by analyzing several important variables for the combustion process.

CFD software is often used for preliminary testing of process behavior and performance required for a new furnace/feed design, design change, or modification of certain characteristics in the combustion process.

The glass industry recognizes ANSYS software as an important CFD simulation tool because of its advantages in enabling the design, testing and integration of technologies, reducing cost, time, and risk, while providing more detailed information.

The software has a user-friendly interface and offers a range of pre-processing, solving, and post-processing capabilities. The version used was the ANSYS 2021 R2. To simulate in ANSYS Fluent, a five-step process is followed (Fernández et al., 2015):

- Design the geometry of the system;
- Generate an appropriate mesh;
- Set up the models to represent the real case;
- Configure the calculation's parameters to run the simulation;
- Results retrieval and visualization.

2.2.1 ANSYS Workspace: Tools and Utilities

Given the intensive use of this tool in this work, Figure 7 shows the main screen of the software, edited to highlight the most important functions.

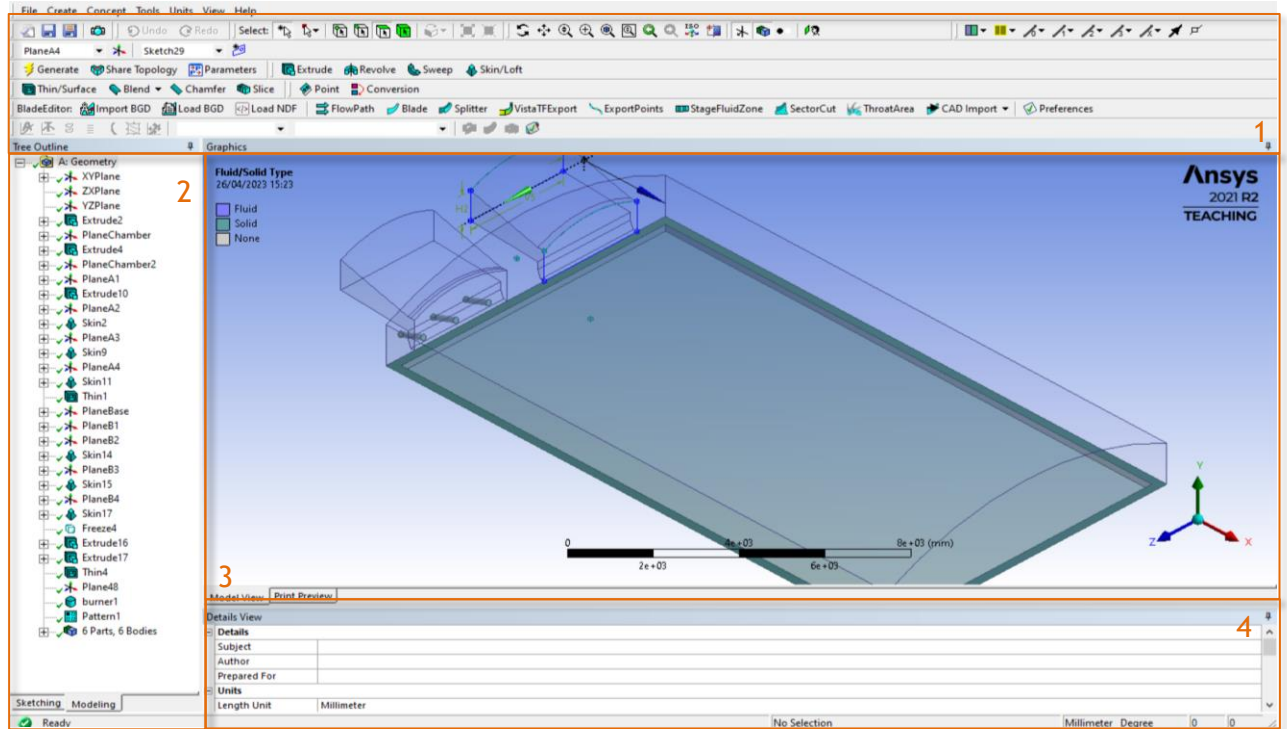


Figure 7 - DesignModeler Tool in ANSYS software (adapted screenshot).

In Figure 7, sector 1 contains the Ribbon, which contains a set of tools for creating and editing the geometry. Sector 2, located on the left side of the screen, shows the Model Tree window, which displays various components such as sketches, features, bodies, and the tools for editing the selected element. Sector 3 provides a 3D view of the geometry model and sector 4 shows the properties window where properties such as the name, material and dimensions can be set.

The mesh generation process is a crucial step and ANSYS software provides a dedicated screen for performing mesh operations (Figure 8). The preparation for the actual simulation is complex because the mesh must be refined at strategic locations, such as the fuel injection area and near the walls, where the largest gradients of the computed variables are expected to occur. This will be discussed in more detail in Chapter 4.

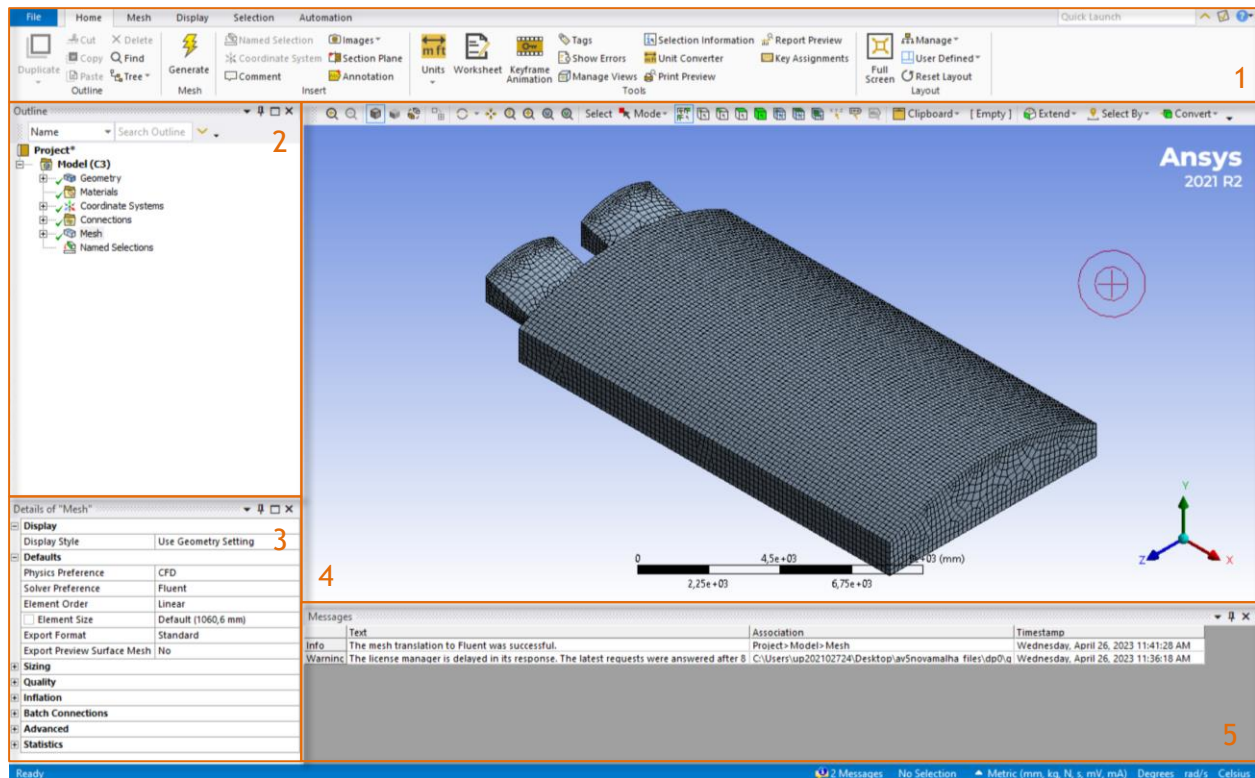


Figure 8 - CFD PrePost in ANSYS software (adapted screenshot).

As can be observed in Figure 8, sector 1 contains the Mesh tab, which contains tools and settings for creating and editing the mesh. Sector 2 shows the outline tree panel, which provides an overview of the entire mesh generation workflow. Sector 3 is where the parameters for the desired mesh can be changed and sector 4 provides a 3D view of it. Finally, sector 5 is normally hidden and displays warnings and errors that may occur after mesh generation.

Figure 9 shows the main window of the software where the simulation is executed, and the results are displayed.

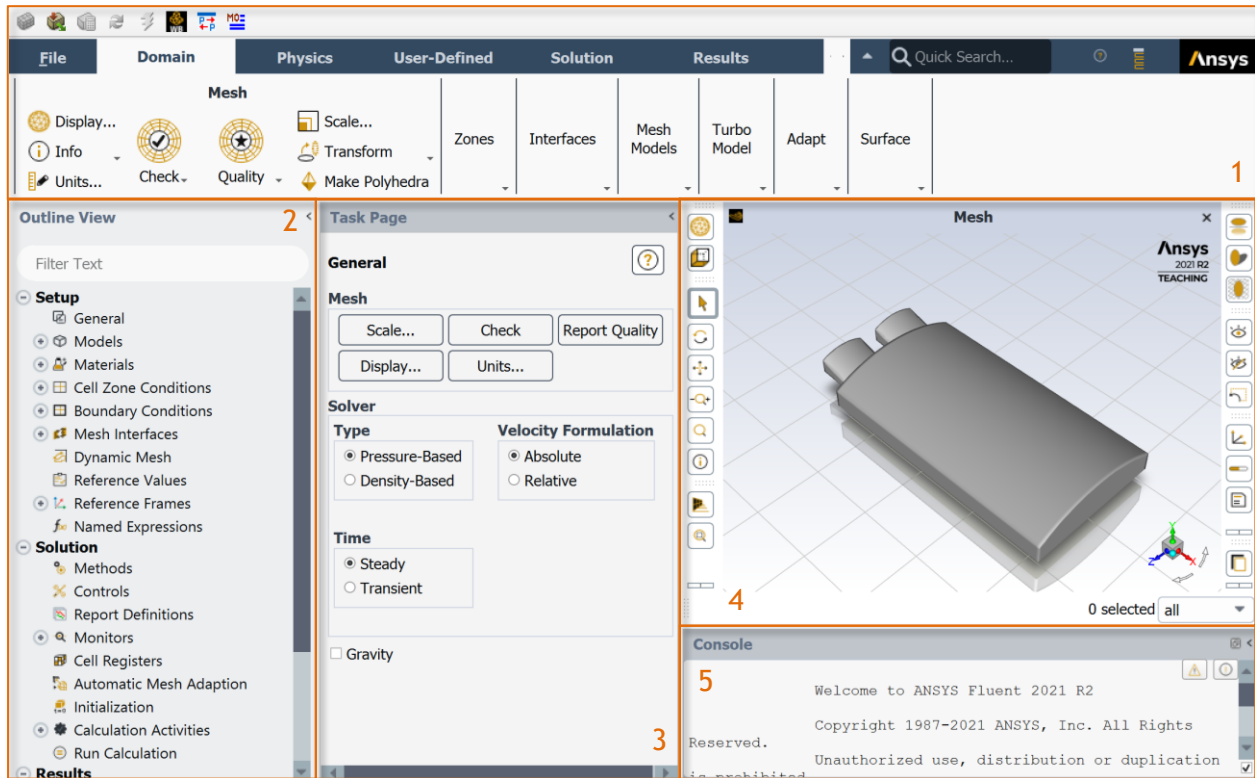


Figure 9 - ANSYS Fluent software (adapted screenshot).

Sectors 1 and 2 in Figure 9 show the ribbon with a visual representation of the simulation setup. Sector 3 includes the task window where the properties and models of the simulation can be specified. Sector 4 displays the graphics window where the user can easily navigate among the many simulation results, and sector 5 provides numerical information about the simulation being run, including any errors that may have occurred.

2.2.2 Numerical Modeling

In numerical combustion studies, to accurately predict combustion characteristics, such as flame shape, temperature and species concentration, the reaction mechanism and radiation model are crucial for accurate prediction of combustion characteristics, together with the conservation equations.

Conservation Equations

A non-premixed flame of natural gas-air is modeled for unsteady state, and the governing equations are written below for a better understanding of the phenomenon.

The continuity equation is given by

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i) = 0 \quad (1)$$

where x_i is the i -component of the position vector, u_i is the i -component of the velocity vector, ρ is the fluid density and t is the time.

The momentum equation is written as:

$$\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial(\rho u_i u_j)}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} \quad (2)$$

where P is the pressure and τ_{ij} corresponds to the viscous stress tensor, given by

$$\tau_{ij} = \mu \left[\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \frac{\partial u_i}{\partial x_i} \delta_{ij} \right] \quad (3)$$

where δ_{ij} is the Kronecker delta and μ is the viscosity coefficient of the fluid.

Equation (4) represents the energy equation:

$$\frac{\partial}{\partial t}(\rho T) + \frac{\partial}{\partial x_i}(\rho u_i T) = \frac{\partial}{\partial x_i} \left(\frac{k}{c_p} \frac{\partial T}{\partial x_i} \right) + S_T \quad (4)$$

where c_p is the specific heat capacity, T is the temperature, k is the conductivity and S_T corresponds to the heat source in the fluid.

For the species conservation, the following equation is solved:

$$\frac{\partial}{\partial t}(\rho Y_l) + \frac{\partial}{\partial x_i}(\rho u_i Y_l) = -\frac{\partial}{\partial x_i}(J_l) + R_l \quad (5)$$

where Y_l is the l -component of the mass fraction, R_l is the l -component of the net generation rate and ∇ is a differential operator. J_l corresponds to the diffusion flux of the component l and is represented by the following equation:

$$J_l = - \left(\rho D_{l,m} + \frac{\mu_l}{S_{c_t}} \right) \frac{\partial Y_l}{\partial x_i} \quad (6)$$

where $D_{l,m}$ is the diffusion coefficient of component l and S_{c_t} is the turbulent Schmidt number (Shakeel et al., 2018; Wen et al., 2021).

Turbulence Modeling

The $k - \varepsilon$ model was selected for this work. This turbulence model utilizes the Boussinesq hypothesis to establish eddy-viscosity, which links the Reynolds stresses ($-\rho u'_i u'_j$) with the average velocity gradients shown in equation (7) and (8).

$$-\rho u'_i u'_j = -\rho \frac{2}{3} k \delta_{ij} + \mu_t \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu_t \frac{\partial u_i}{\partial x_i} \delta_{ij} \quad (7)$$

where

$$\mu_t = \rho C_\mu \frac{k^2}{\varepsilon} \quad \text{and} \quad C_\mu = 0.09 \quad (8)$$

The equations for k and ε transport involve the turbulent kinetic energy and its rate of dissipation. These equations are derived based on the assumption of isotropy as expressed:

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(\rho u_i k) = \frac{\partial}{\partial x_i} \left(\frac{\mu_t \partial k}{\sigma_k \partial x_i} \right) + G_k - \rho \varepsilon \quad (9)$$

$$\frac{\partial}{\partial t}(\rho \varepsilon) + \frac{\partial}{\partial x_i}(\rho u_i \varepsilon) = \frac{\partial}{\partial x_i} \left(\frac{\mu_t \partial \varepsilon}{\sigma_\varepsilon \partial x_i} \right) + C_1 \frac{\varepsilon}{k} G_k - C_2 \rho \frac{\varepsilon^2}{k} \quad (10)$$

where

$$G_k = \mu_t \left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right) \frac{\partial u_i}{\partial x_i}, \quad C_1 = 1.44, \quad C_2 = 1.92, \quad \sigma_k = 1.00 \quad \text{and} \quad \sigma_\varepsilon = 1.30. \quad (11)$$

The $k - \varepsilon$ model is effective to predict the flow behavior in many turbulent scenarios, but it does have some limitations (Galletti et al., 2013; Guessab et al., 2013). This turbulence model is more accurate the inner core regions of the flow. This is because, in regions close to the boundaries (such as the walls), the turbulence level changes significantly, causing the models to become less accurate. To address this issue, a special approach is used in the near-wall region called the wall-function approach, which uses semi-empirical formulas to bridge the gap between the wall and the fully turbulent region and determine the values of variables in this region. The Standard Wall Functions model was used. The near-wall region's velocity, temperature, and turbulent quantities can be determined using wall functions instead of solving the governing equations. The turbulent kinetic energy in the region close to the wall is determined using the transport equation and the following boundary condition (Ishii et al., 2002):

$$\frac{\partial k}{\partial n} = 0 \quad (12)$$

Combustion Modeling

A reaction mechanism is necessary to calculate reaction rates for species conservation equations, but it can be very complex when dealing with a large number of species and parallel reactions. In the case of the fuel used in this study, which is a mixture of many gases, it is challenging to determine a detailed reaction mechanism. To solve this problem, a combustion model called the mixture fraction/Probability Density Formula (PDF) can be used, which involves solving a conserved scalar to derive individual species concentrations. The conserved scalar is defined as the mixture fraction, f :

$$f = \frac{Z_k - Z_{ko}}{Z_{kf} - Z_{ko}} \quad (13)$$

where Z_k is the mass fraction of species k and subscripts f and o are the fuel and oxidizer stream conditions at the inlet. It is conserved and varies between 0 (at the oxidizer inlet) and 1 (at the fuel inlet). The transport equation for the mixture fraction below can be used to determine its value at any point in the system:

$$\frac{\partial \rho \bar{f}}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i \bar{f}) = \frac{\partial}{\partial x_i} \left(\frac{\mu_t}{\sigma_t} \frac{\partial \bar{f}}{\partial x_i} \right) \quad (14)$$

The connection between the current levels of species concentrations and mixture fraction in a system can be determined based on the system's chemical description. In non-premixed combustion with turbulence, the speed of turbulent mixing is much slower than the speed of fuel conversion. One approach commonly used in modeling turbulent non-premixed combustion is assuming fast chemistry. There are two options for describing system chemistry without knowledge of the reaction mechanism. The first option, called the flame sheet approximation, assumes infinitely fast chemistry where fuel and air never coexist, and a straight-line relationship exists between mixture fraction and species mass fractions. However, this approach is limited to single-step reactions. The second option, the equilibrium assumption, does not require reaction stoichiometry and can predict intermediate species formation and dissociation effects by minimizing Gibbs free energy. In this type of combustion, the thermochemical state of the mixture is a function of the mixture fraction and enthalpy, h , as follows:

$$\phi_i = \phi_i(f, h) \quad (15)$$

where ϕ indicates an instantaneous species concentration, temperature, or fluid density.

When considering fluctuations over time, a joint probability density function (PDF) of f and h is needed. However, calculating this PDF is not feasible in engineering applications. If heat losses play little impact on turbulent enthalpy fluctuations, $P = P(f)$ is assumed. With this assumption, the Favre-averaged values of ϕ can be obtained by

$$\bar{\phi}_i = \int_0^1 P(f) \phi_i(f, h) df \quad (16)$$

The probability density function's shape depends on the type of turbulence fluctuations encountered. These functions are used to calculate mean values from instantaneous values. There are two mathematical functions available in Fluent for describing the shape of the PDF. The first is the double δ function, which is computationally less intensive and the second is the β -function (Stockwell et al., 2001).

Radiation Modeling

The Radiative transfer equation (RTE) for an absorbing, emitting, and scattering medium at position r and direction s is expressed as:

$$\frac{dI(r, s)}{ds} + (\alpha + \sigma_s) I(r, s) = \frac{\alpha n^2 \sigma T^4}{\pi} + \frac{\sigma_s}{4\pi} \int_0^{4\pi} I(r, s) \varphi(s, s') d\Omega' \quad (17)$$

where I is the radiative intensity, σ_s is the scattering coefficient, α is the absorption coefficient, φ is the scattering phase function and Ω is the solid angle. Both the scattering coefficient and the absorption coefficient affect how much the radiation intensity changes. When considering radiation in semi-transparent media, as in the glass case, the refractive index, n , is important. Another form of equation (17) is the following one:

$$\frac{dI(r,s)}{ds} = -\beta I(r,s) + S(r,s) \quad (18)$$

where $\beta = (\alpha + \sigma_s)$ is the extinction coefficient and $S(r,s)$ corresponds to the radiation source term appearing in the conservative energy equation, written as:

$$S(r,s) = S_{\text{radiation}} = \alpha I_b + \frac{\sigma_s}{4\pi} \int_0^{4\pi} I(r,s) \varphi(s,s') d\Omega' \quad (19)$$

where $I_b = \frac{\sigma T^4}{\pi}$ is black body radiative intensity. Thus, when the radiant heat flux, $Q_{\text{rad}} = \sigma(T_{\text{max}}^4 - T_{\text{min}}^4)$ is large compared to the heat transfer rate due to conduction or convection, this parameter should be included in the simulation. This phenomenon occurs normally at high temperatures (Bidi et al., 2008; Shakeel et al., 2018).

To be more precise, the radiation model used in this combustion process was the *Discrete Ordinate Method* (DOM). The DOM approach utilizes a limited set of predetermined angles that correspond to specific vector directions in the global Cartesian system (x, y, z) and uses these directions to solve the RTE. This involves converting the original equation into a transport equation for radiation intensity in the spatial coordinates (x, y, z) and solving multiple transport equations for each fixed direction s . This model considers RTE in the direction s as a field equation and is described as:

$$\nabla \cdot (I(r,s)s) + (\alpha + \sigma_s)I(r,s) = \alpha n^2 \frac{\sigma T^4}{\pi} + \frac{\sigma_s}{4\pi} \int_0^{4\pi} I(r,s) \varphi(s,s') d\Omega' \quad (20)$$

The RTE for the spectral intensity $I_\lambda(r,s)$ can be expressed as:

$$\nabla \cdot (I_\lambda(r,s)s) + (\alpha_\lambda + \sigma_s)I_\lambda(r,s) = \alpha n^2 I_{\lambda b} + \frac{\sigma_s}{4\pi} \int_0^{4\pi} I_\lambda(r,s) \varphi(s,s') d\Omega' \quad (21)$$

The given equation involves the wavelength (λ), the spectral absorption coefficient (α_λ), and the black body intensity ($I_{\lambda b}$) according to the Planck function. The scattering coefficient, scattering phase function, and refractive index are assumed to be constant regardless of wavelength (Bidi et al., 2008).

3 Furnace Characterization

In this project, the behavior of an end port regenerative furnace is studied with the goal to reduce the flue gases released and the energy consumption. Several parameters, such as the NO_x , CO and CO_2 formation, energy usage, flame interaction and maximum furnace temperatures will be investigated to improve the combustion chamber efficiency.

To carry out this investigation, a baseline model study of the furnace currently installed at BA Glass Avintes is undertaken by analyzing the performance of the CC in certain conditions. In the next step, this scenario is used as a reference case for the calculations varying the parameters that will be studied. In this Chapter, a computer model is generated for the combustion chamber (Figure 10), based on the technical drawings and information provided by the host company.



Figure 10 - Furnace facility outside and inside views.

The studied combustion chamber is characterized in terms of fuel and oxidizer compositions, dimensions, material, air to gas ratio, temperatures, and flow rates. The combustion tests carried out were representative of the facility shown in Figure 10.

3.1 Material and Dimensions

The drawings provided by BA Glass Avintes included the materials and their properties used in the refractories of the furnace. As shown in Figure 11, the material used in the crown and the other walls are silicon and fused cast AZS (Alumina-Zirconia-Silica), respectively, which can resist to temperatures higher than 1500°C .

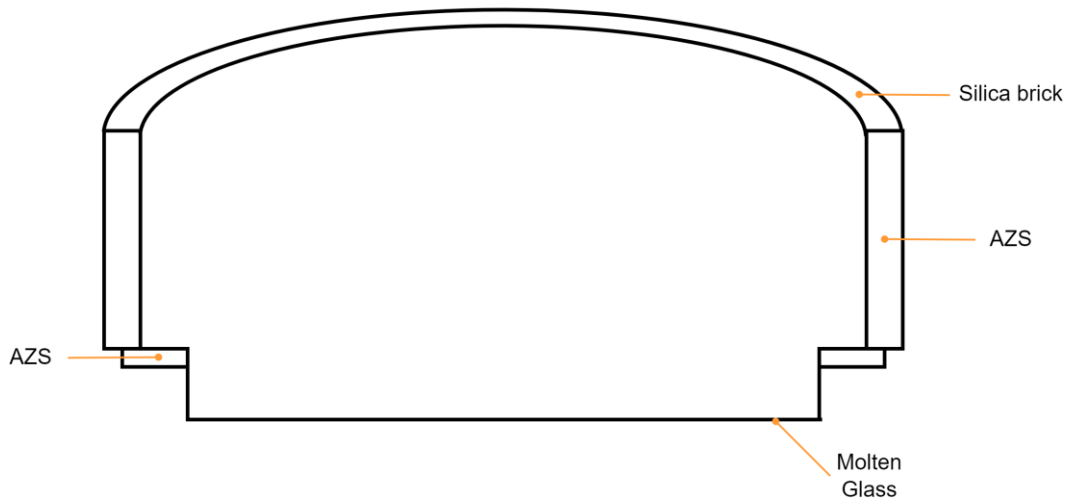


Figure 11 - Combustion chamber materials.

Table 1 exhibits the bulk density, the cold crushing strength, and the thermal conductivity of the material.

Table 1 - Combustion chamber material properties.

	Silica brick	Fused cast AZS
Bulk density (g/cm ³)	1.83	3.75
Cold Crushing Strength (MPa)	40	>300
Thermal Conductivity (W/m K) at 1400°C	2.1	5.1

The technical drawings were provided by BA Glass but are not shown here because these are confidential documents. AutoCAD software was used to represent the frontal, lateral and superior views of the chamber, as shown in Figures 12, 13 and 14. Not all the dimensions were allowed to be represented due to confidentiality reasons. The actual CC has two ports, and five burner nozzles are installed in both sides but only three are in operation. For this base-case simulation, the ports are only represented in the chamber's right side with a time cycle of approximately 30 min, where the pre-heated air enters in the right port and the flue gases exit through the left one. Another assumption done was considering negligible wall thicknesses. Figure 12 represents the superior view of the CC.

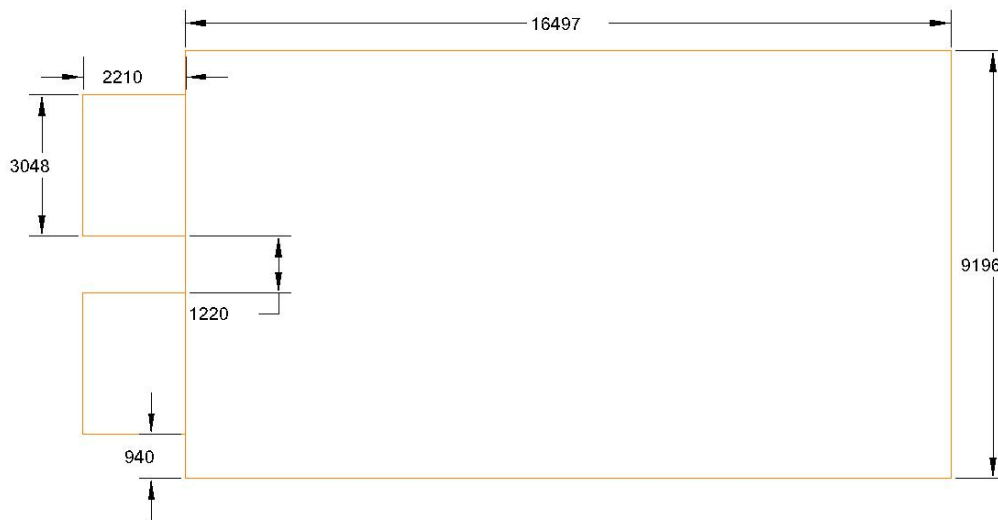


Figure 12 - Superior view of the combustion chamber. The length shown is in millimeters.

Figure 13 shows the frontal view of the CC and its dimensions, where the burners are not drawn. However, they are distributed on the right side of the chamber and the distance between them is 909 mm.

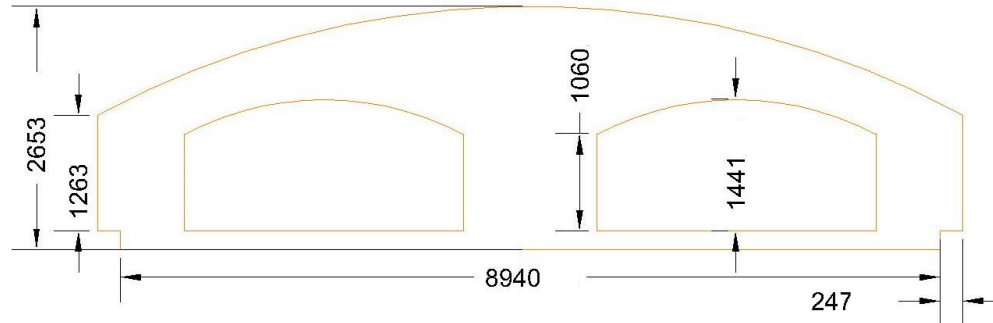


Figure 13 - Frontal view of the combustion chamber. The length shown is in millimeters.

In Figure 14, the upward angle of the burner port is 5° and the nozzle is positioned 18.9 mm above the base of its wall. The radius of the nozzles is 80.2 mm and its length is 5 times its diameter, which corresponds to 802 mm. Furthermore, its inclination was considered the same as the downstream wall.

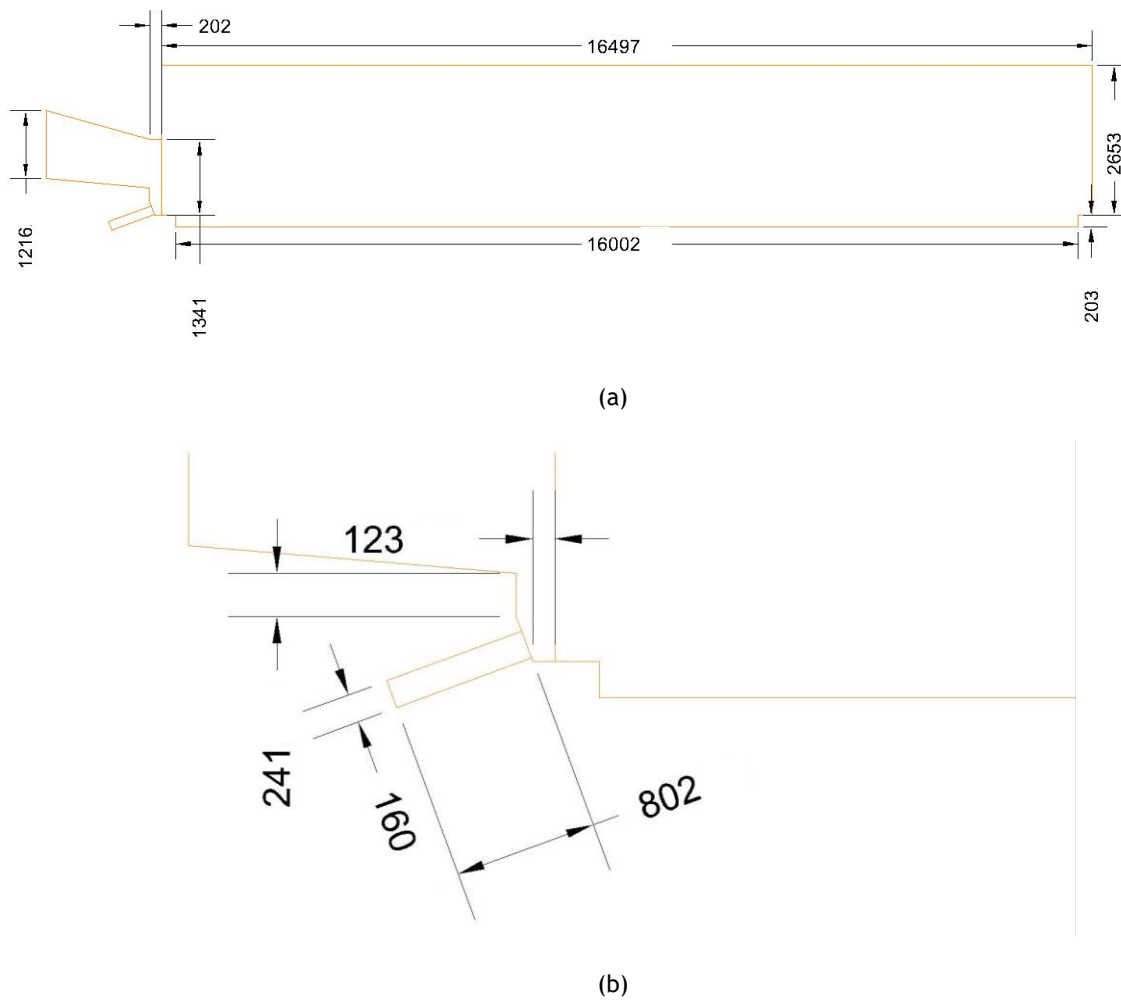


Figure 14 - (a) Lateral view of the combustion chamber; (b) Close up of the burner. The length shown is in millimeters.

3.2 Natural Gas and Air Composition

One of Redes Energéticas Nacionais (REN)'s customers is BA Glass and the fuel provided by them is natural gas. The fuel composition corresponding to April 2023 is presented in Table 2.

Table 2 - Natural gas composition provided by REN (Sistema de Informação de Mercados de Energia, 2023).

Component	mol %
CH ₄	95.27
C ₂ H ₆	3.69
C ₃ H ₈	1.04

The low heating value (LHV) of this mixture corresponds to 10.63 kWh/Nm³, available in Sistema de Informação de Mercados de Energia (2023). Butane and pentane are not considered for the mixture composition due to their residual values.

The air that feeds the furnace is captured from the atmosphere and the volumetric composition of the main components is provided in Table 3.

Table 3 - Atmospheric air composition.

Component	vol %
O ₂	20.56
N ₂	77.60
H ₂ O	1.84

For this case study, H₂O was not considered for the atmospheric air composition.

3.3 Gas and Primary Air

To simulate the combustion in the CC, the flow rates for both the fuel and the preheated air from the regenerator must be known. After processing the data provided by BA Glass, the volumetric flow of natural gas corresponds to an estimated value of 1419 Nm³/h and the preheated air flow to 19152 Nm³/h. Thus, the stoichiometric air/gas ratio is 13.5 for both sides of the regenerator, with a target oxygen concentration in the dry flue gas of 2.5%. This allows to determine the mass flow rate introduced in both inlets of NG and air, 0.1069 kg/s and 6.2987 kg/s, respectively. However, the air flow rate depends on the draft capacity of the furnace, which is, typically, 410 tons per day. Into the port-neck inlet the preheated air is supplied at a temperature of 1450 °C and the natural gas enters the burners at 28 °C. From the data of the computer in the control room of the B&F Department, the flue gases temperature at the outlet is about 1600 °C.

Within the combustion chamber and chimney, there are points where temperature, and composition of the flue gas are measured. The dimensions of the visible part of the flame were visually measured by the operators through inspection windows and installed cameras. The actual length of the flame was measured from the front of the combustion chamber where the throat is installed as seen in Figure 15.



Figure 15 - Flame in the combustion chamber.

Generally, the dimensions of the flame are between half and 2/3 of the combustion chamber's length, so its value is around 8 to 10 m. Table 4 summarizes all data collected on the studied furnace.

Table 4 - Operating conditions for air-NG run in the initial case.

Parameter	Value
NG flow rate	1419 Nm ³ /h
NG temperature	28 °C
Air flow rate	19152 Nm ³ /h
Air temperature	1450 °C
Air/gas ratio	13.5
Oxygen flow rate	4022 Nm ³ /h
Flue gas temperature	1600 °C
O ₂ in flue gas (port)	2.5%
O ₂ in flue gas (chimney)	9%
CO ₂ in flue gas (chimney)	8.17%
NO _x in flue gas (chimney)	708 mg/Nm ³

The data relating to the chimney was taken from a characterization of the gaseous emissions, since there are no measurements of the same pollutants at the outlet of the combustion chamber. Therefore, these values are used as reference data. In addition, the value for oxygen

concentration in the chimney is higher than the one leaving the combustion chamber directly, due to the penetration of stray air.

4 CFD Simulations

4.1 Geometry and Mesh Generation

The geometry was created in ANSYS DesignModeler, including the combustion chamber and the burner nozzles, as seen in Figure 16, matching closely the real sizes of the CC.

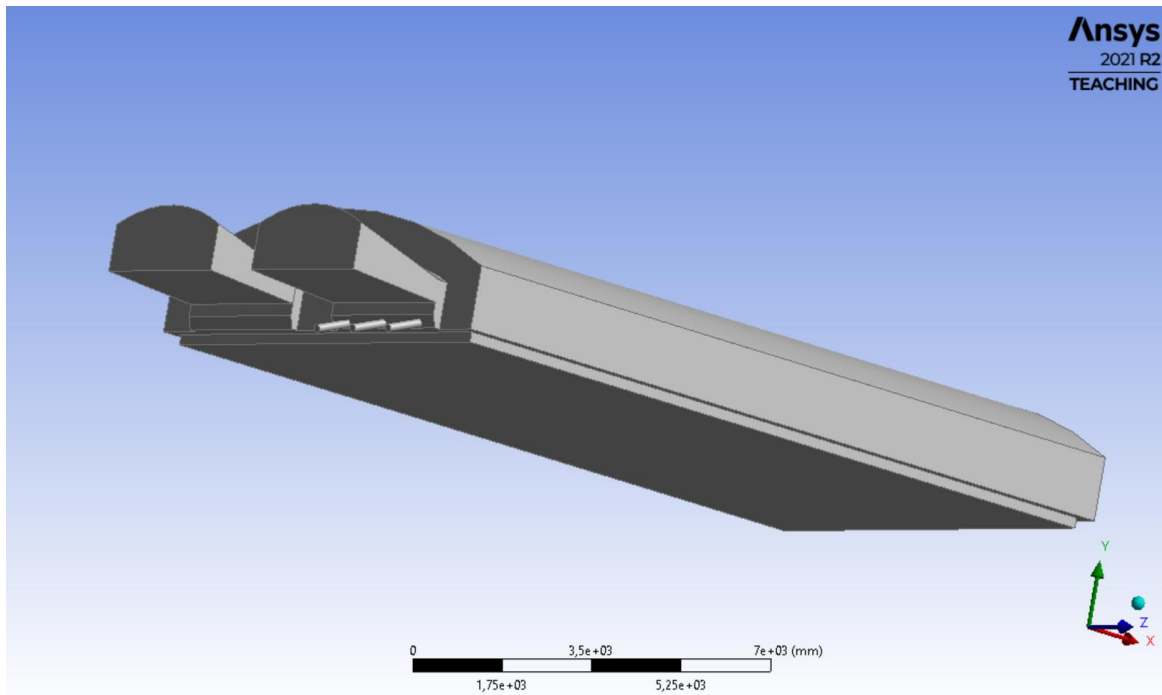


Figure 16 - Combustion chamber geometry.

When creating the combustion chamber mesh, a minimum number of cells must be considered for the results to be accurate. However, a very fine 3D mesh may result in excessive computational overhead, while a coarse mesh significantly may affect the accuracy of the simulation. There are regions that require more attention in meshing the geometry, such as the boundary layers near the walls of the combustion chamber, where significant gradients occur. Fuel injection zones, and regions where combustion is expected to occur were also analyzed with more detail. This is critical, for example, for detecting reaction fronts, flame propagation, and the interaction between the flame and the flow fields.

The mesh used for the combustion chamber simulation is an unstructured mesh consisting of polyhedral elements. It was created using a hybrid mesh creation process that includes manual refining and automated meshing techniques. The total size of the mesh includes 118147 elements distributed over the entire combustion chamber, with higher mesh resolution near the walls and fuel injection regions to capture the physics of the boundary layer. Mesh quality was prioritized, and steps were taken to ensure well-formed parts. The worst cells will have an orthogonal quality closer to 0, with the best cells closer to 1. The minimum level of

orthogonality required for all cell types should exceed 0.01, with an average value that is significantly higher, 0.2, which was the value obtained for the CC mesh. The maximum aspect ratio is 17.8, which is high, but acceptable in inflation layers. To represent the inlet, outlet and wall surfaces, the appropriate boundary conditions were defined. In Figure 17, a view of the final mesh used for the simulations is presented in different views.



Figure 17 - Mesh representation in different views.

The mesh used in this combustion chamber simulation provides a well-refined representation of the geometry and is expected to properly capture the essential characteristics of the flow and combustion processes.

4.2 Simulation Setup

The main objective of this work is to analyze the flow, combustion, and emission characteristics to improve combustion efficiency while reducing the formation of NO_x and other pollutants with different levels of oxygen enrichment in the intake air stream.

In the present study, the CC was modeled using a 3D computational domain, as previously described. The set of governing equations for continuity, momentum, energy, turbulence, combustion, and radiation were numerically solved with proper boundary conditions. "Pressure-

based" and "transient" state were chosen for the solver type, since the initial simulations considering steady state showed that the solution didn't converge. Turbulence modeling within the structure was done using the realizable $k-\varepsilon$, with the Standard Wall Functions Model.

For the boundary conditions on the walls of the furnace, the temperature of the glass surface is 1350 °C and its emissivity is 0.92. Steel was assumed to be the material of the walls chamber with an emissivity of 0.59.

A non-premixed combustion was chosen for the species model, and the process was considered non-adiabatic, and the model was operating at atmospheric pressure, with a fuel stream rich flammability of 0.1. The fuel was modeled as a mixture of CH_4 (95.27% by mol), C_2H_6 (3.69% by mol) and C_3H_8 (1.04% by mol) and for the base case, the oxidizer had 21% of O_2 and 79% of N_2 , as written in Tables 2 and 3.

At the flow inlet, a mass flow rate in boundary conditions was established for the fuel as 0.1069 kg/s. The temperature was set at 28 °C and the hydraulic diameter of each burner was set at 160.4 mm. For the oxidizer, the mass flow rate is 6.2987 kg/s, and the temperature is 1450 °C, as already mentioned. The boundary condition for the combustor outlet was set to a pressure outlet at atmospheric conditions (i.e., zero-gauge pressure).

While convective terms are discretized using the first or second-order upwind approach, the pressure equation is discretized using a second order scheme. Pressure-velocity coupling is ensured using the semi-implicit technique for pressure-linked equations (SIMPLE) algorithm. This information, as well as the under-relaxation factors (URF), are shown in Table 5.

Table 5 - Under-relaxation factors and convective scheme.

URF		Convective Scheme	
Pressure	0.3	Solver Type	Pressure based
Density	1	Viscous model	Realizable $k-\varepsilon$
Momentum	0.7	Momentum	Second order upwind
Turbulent viscosity	1	Pressure-velocity coupling	SIMPLE
Temperature	1	Pressure model	Second Order
Energy	1	Energy	Second order upwind
Turbulent kinetic energy	0.8	Turbulent kinetic energy	First order upwind

Turbulent dissipation rate		0.8	Turbulent dissipation rate		First order upwind
Pollutant no		1	Pollutant no		Second order upwind
Radiation model		1	Radiation model		First order upwind
Mean mixture fraction		1	Mean mixture fraction		Second order upwind
Mixture fraction variance		0.7	Mixture fraction variance		Second order upwind

In the discretization of the convective term, second order upwind is used in several equations but to enhance the stability of the numerical methods in some cases the upwind scheme is used, despite its lower order of accuracy.

To study the impact of different O_2 concentrations in the combustion process and pollutants emissions, a series of air-natural gas runs were carried out under various operating conditions. Table 6 presents the operating conditions for each run, highlighting the variations in mole fraction of O_2 .

Table 6 - Operating conditions for air-NG run in different cases.

	O_2 Mole fraction	Q_{oxidizer} (m^3/h)	m_{oxidizer} (kg/s)	Q_{O_2} (m^3/h)	Q_{N_2} (m^3/h)
Baseline	0.21	19152	6.2987	4022	15130
Case 2	0.25	16087	5.2909	4022	12066
Case 3	0.30	13406	4.4091	4022	9384
Case 4	0.35	11491	3.7792	4022	7469
Case 5	0.40	10055	3.3068	4022	6033

The mole fraction of O_2 was systematically varied across the runs, ranging from 21% to 40% to assess the variation of several parameters such as the maximum flame temperature and mass fractions of pollutants (CO , CO_2 , and NO_x) at the outlet. The aim was to maintain the volumetric flow rate of oxygen entering the combustion chamber, since $4022 m^3/h$ of O_2 is an adequate value to allow an efficient combustion and, consequently, reducing the volumetric flow rate of

nitrogen to obtain the chosen O_2 mole fraction. The data provided in Table 6 is described in Appendix A.

4.3 Results

The numerical results presented include the velocity field, energy usage, maximum temperature in the combustion chamber (maximum temperature in the flame), the temperature at outlet and the mass fraction of pollutants. Due to transient nature of the process, the variables were monitored along time and the results were exported to Microsoft Excel and a data analysis was performed. In this technical analysis it was necessary to select the time interval in which the solution showed a quasi-periodic behavior and obtain the average, amplitude, and standard deviation values for each variable.

It is necessary to consider that the numerical results of this dissertation do not reproduce the experimental values with great accuracy due to the simplicity of the chosen combustion model. The main goal of this preliminary investigation is to predict the tendency and the behavior of the analyzed parameters with the variation of O_2 concentration at inlet. Bělohradský et al. (2014) study was used to compare with the results obtained.

In the initial simulations, some numerical experiments were performed with different time-steps (0.05 s and 0.1 s) to find out which time step and maximum number of iterations per time step are adequate. Figure 18 shows the transient behavior of the CO_2 mass fractions for a time interval that corresponds to approximately 2 residence times in the furnace.

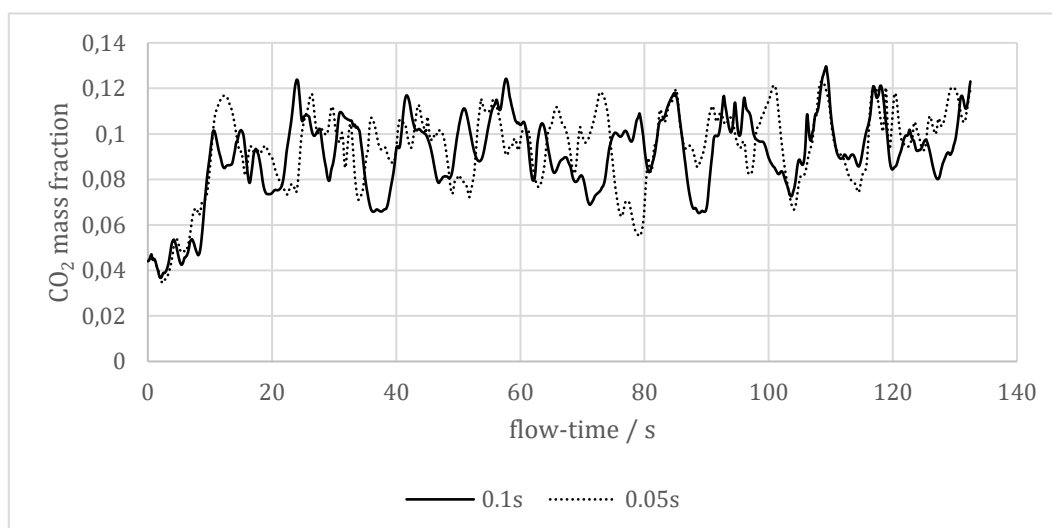


Figure 18 - Variation of CO_2 mass fraction at the outflow as function of time for 2 different values of the time-step.

From Figure 18, it is clear that the behavior is similar for both time steps. The time series also show that the transient effects are not disappearing at large times, and the system does not reach a steady-state condition. The solution gradually changes over the initial 10-20 s, and afterwards a quasi-cyclic behavior is found for both time steps. Therefore, to reduce the required computational times, the larger time step (0.1s) was chosen for the next simulations with 10 iterations per time step. To discuss the numerical results, a data analysis was done extracting the average and standard deviation of the values provided by the graphics.

4.3.1 Velocity Field

In this section, to analyze the flow field and the possible occurrence of dead volumes in the CC, instantaneous velocity vectors were plotted in plane XY crossing the inlet and outlet boundaries after 2-time constants. Baseline case and case 5 at higher O_2 concentration (lower inlet mass flow rate) are presented in Figure 19.

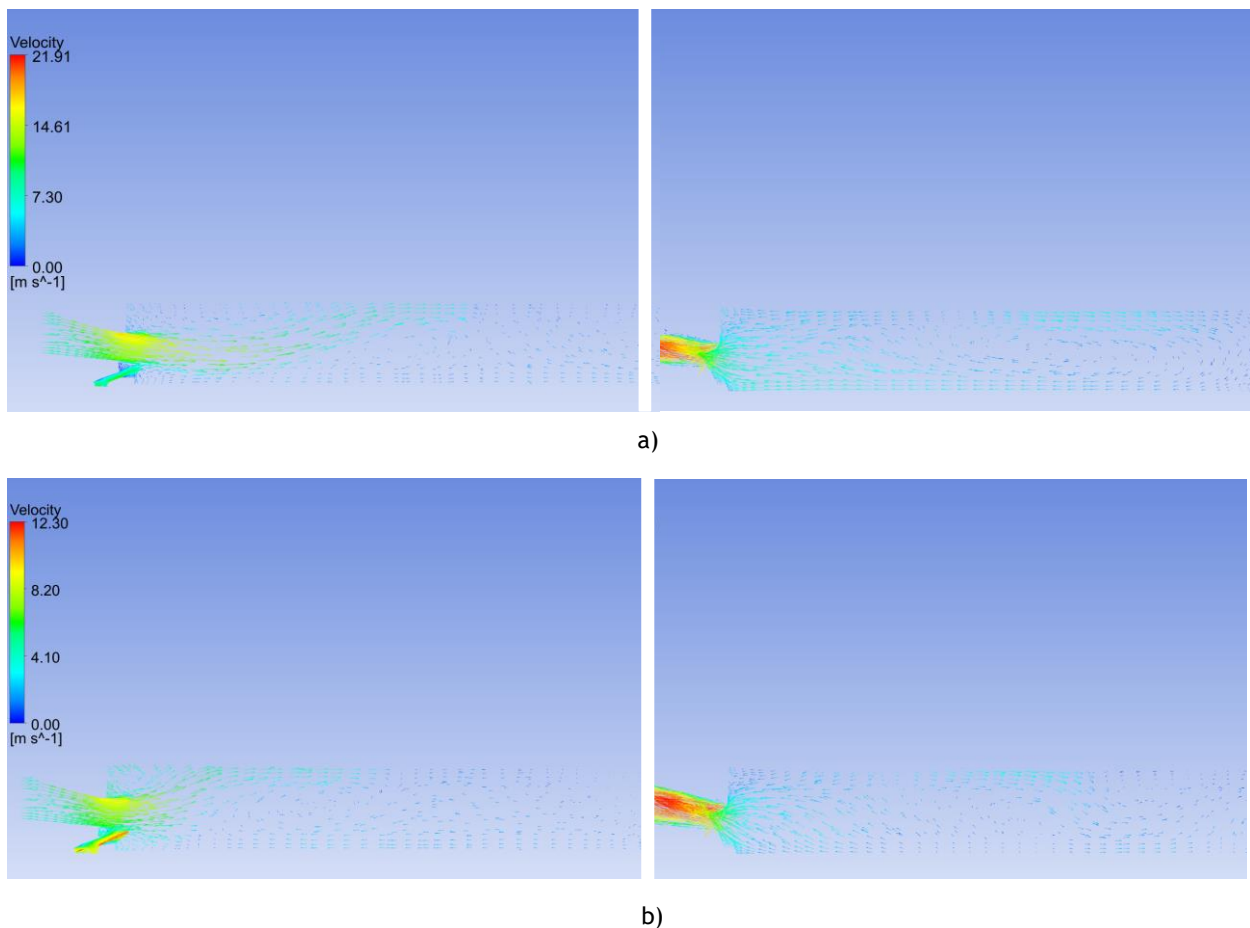


Figure 19 - Velocity vectors at planes crossing the inlet and outlet boundaries for different inlet oxygen concentrations a) 21%; b) 40%

As expected, the velocity magnitude decreases since the air mass flow rate in case 5 is lower. Velocity and mass flow rate are directly proportional when the other factors remain constant.

Therefore, when enriching O_2 in the inlet while maintaining the oxygen mass flow rate due to the reduction in nitrogen mass flow rate, the velocities in the CC will decrease. The velocity decrease will increase the residence time of the flows in the CC and consequently oxidation reactions can take place for a longer duration, facilitating the conversion of pollutant.

It can also be seen that there are dead zones, especially at the edges and corners of the CC and in the recirculation zones. These areas affect turbulence and can result in incomplete combustion and increased emissions. The velocity fields for the other cases simulated are shown in Appendix B.

4.3.2 Total Heat

The total heat released by the combustion reaction is an important variable to analyze due to the opportunity of increasing the energy provided to the glass. Figure 20 shows the numerical results of this variable for the different inlet O_2 concentrations.

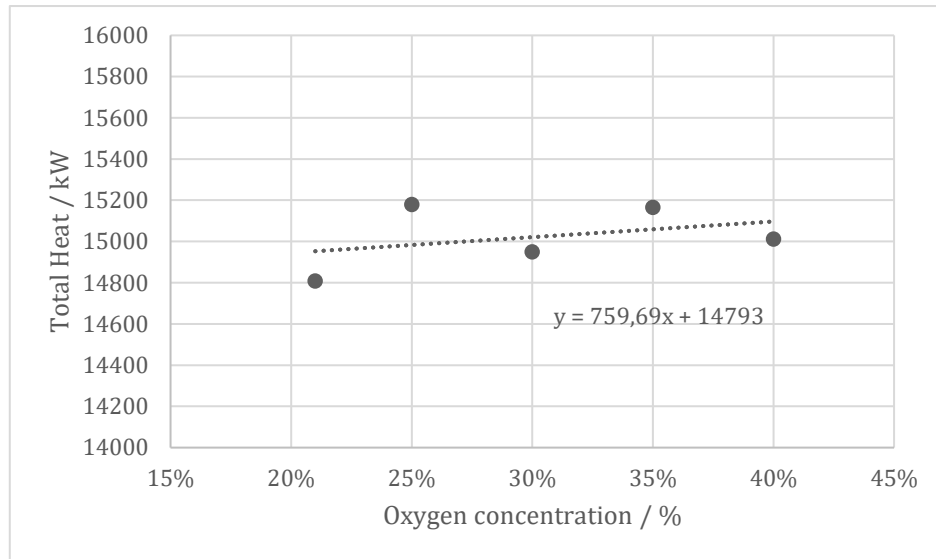


Figure 20 - Effect of inlet oxygen concentration on the total sensible heat.

The values vary slightly between 14808 kW and 15179 kW, and they oscillate. However, the tendency line is increasing, which means a slightly more efficient energy release. This can be explained by several factors, such as the reduced inert gas dilution, which leads to the increased flame temperature (as it will be explain later) and consequently to the enhanced combustion efficiency. The presence of enriched combustion air with oxygen in the inlet increases the flame temperature, which is directly correlated with the energy released during combustion process. Thus, with less N_2 mass flow rate in the inlet air, the reaction will be more efficient, and more energy will be available to the glass melting because it doesn't spend that much energy in heating the inert gas.

4.3.3 Temperature

4.3.3.1 Maximum and Flame Temperature

Figure 21 shows the effect of different feed oxygen mole fractions on the maximum temperature in the CC. This temperature corresponds to a specific point of the combustion chamber within the flame and vary in magnitude and location with time due to the non-stationary flow field. Note that, these values do not correspond to the average temperature of the flame, which is significantly lower, as seen in Figure 22. The results of each graph were obtained through an average of the transient values obtained in ANSYS Fluent, and they are detailed in Appendix C.1.

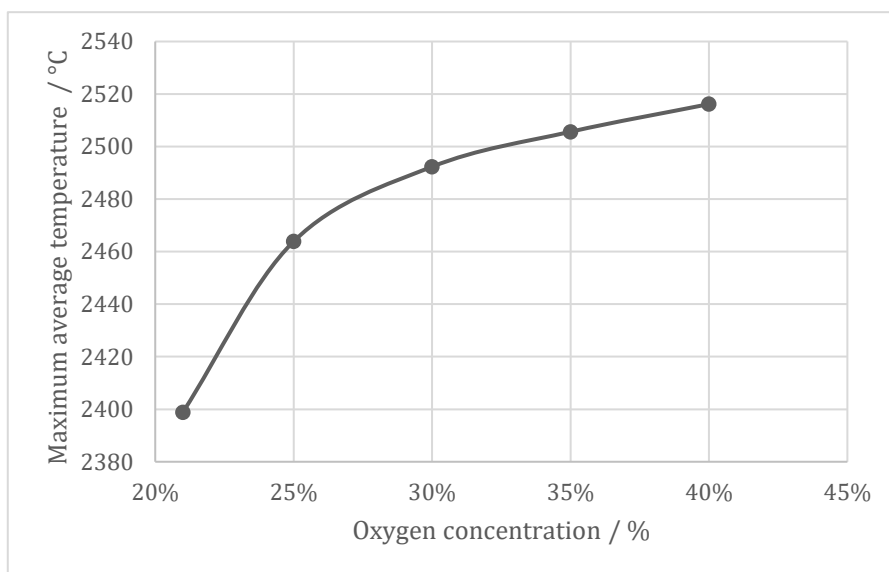


Figure 21 - Effect of inlet oxygen concentration on the maximum averaged temperature in the flame.

As expected, the maximum temperature in the CC increases as the oxygen concentration increases which leads to a higher efficiency of the combustion, ranging from 2399°C to 2516°C. These values are higher than expected, but these can be explained by the fact that the non-premixed combustion model may not capture fine details of the process and these values are local and correspond to the maximum values. The increase of the temperature in the CC is due to the reduction of N₂ flow rate, which leads to a more oxygen-rich environment and a more complete combustion of the fuel, increasing the energy release as well.

To analyze in more detail the flame temperature field for different inlet oxygen content, a surface contour plot in plane XY is shown in Figure 22.

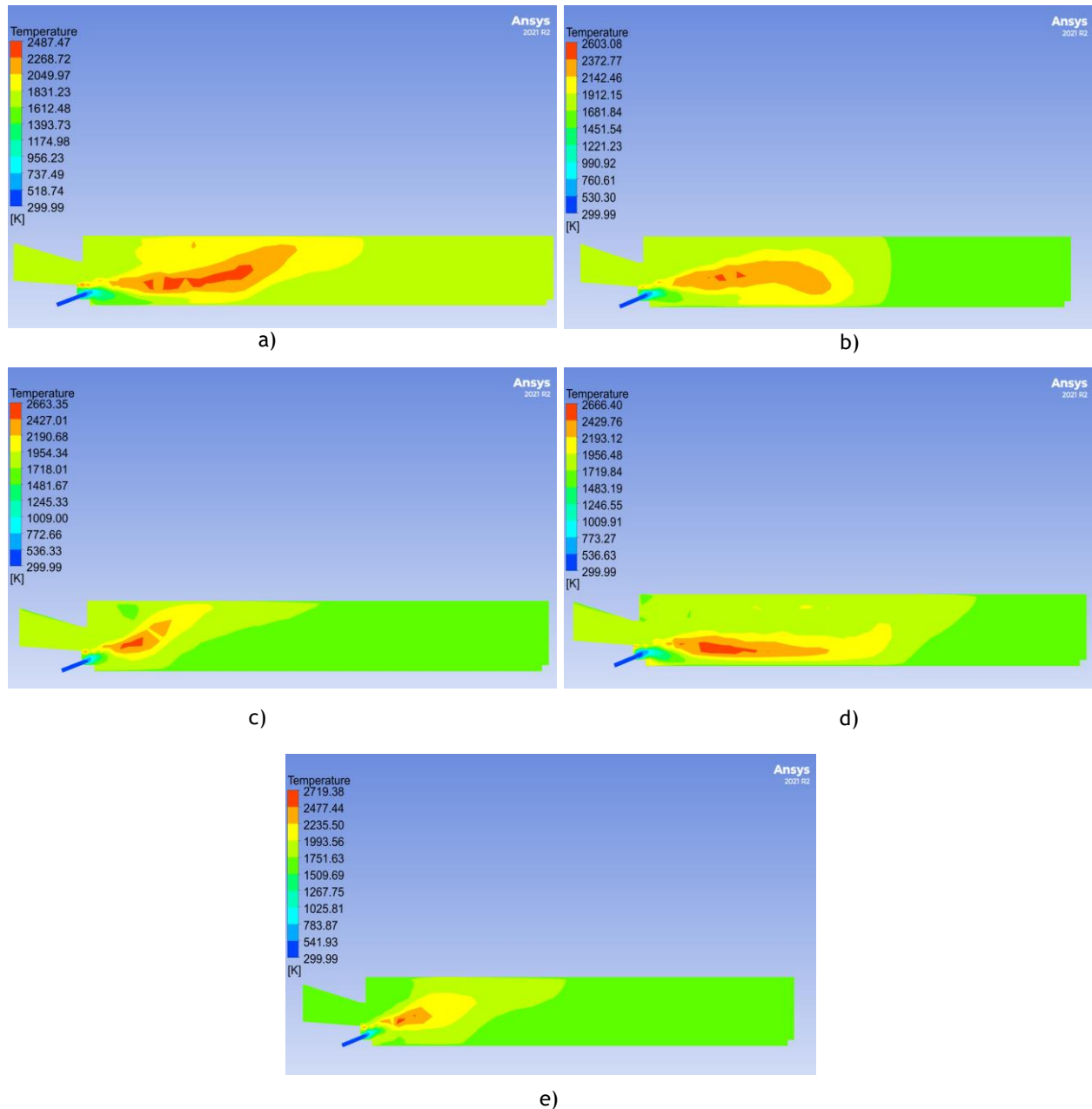


Figure 22 - Instantaneous temperature contours for different inlet oxygen concentrations: a) 21%; b) 25%; c) 30%; d) 35%; e) 40%.

The flame in the combustion chamber of the furnace under study oscillates with time. Figure 22.a) provide a validation of the base-case simulation since the flame temperature and length are similar to the data observed in the real combustion chamber. An interesting observation was made regarding the impact of oxygen enrichment on flame length, and it was noticed that when oxygen concentration introduced into the combustion airstream increased, the flame length became shorter, and it can also be explained due to the smaller velocities at higher O_2 concentrations. Case 4 shows to be an exception, having a higher flame length than case 3. Due to the unsteady nature of the flow and flame dynamics this might correspond to a specific time in which the flame is more aligned with the chamber, thus being longer.

Given the increase in the temperature scale, the flame reveals a brighter appearance at higher O_2 concentrations compared to the initial case, with atmospheric air fed to the CC. The reason for this is that as the oxygen content in the mixture increases and the N_2 flow rate decreases, the flame length becomes shorter, and the flame becomes more intense.

4.3.3.2 Flue Gas Temperature

Figure 23 shows how the average temperature of the flue gas varies as the oxygen content changes, which data can be found in Appendix C.1.

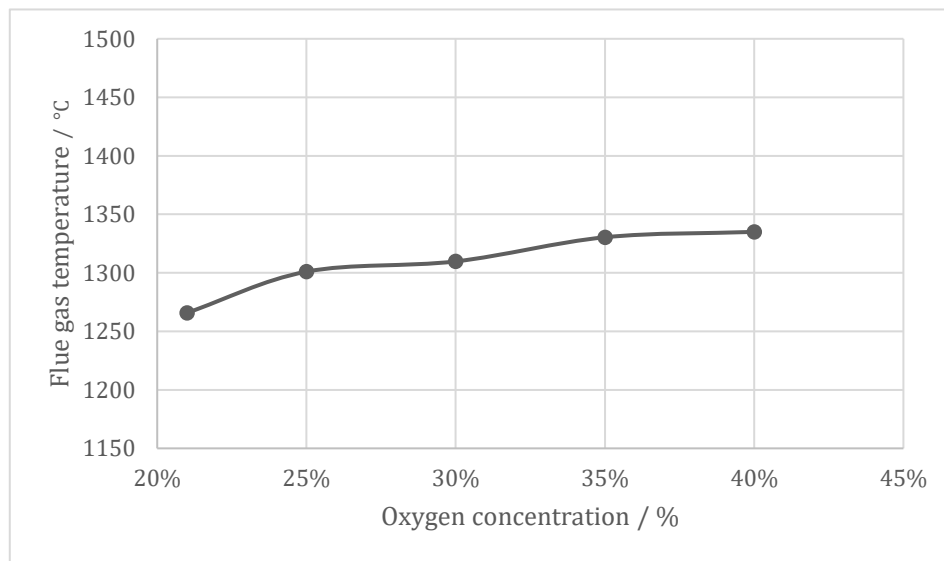


Figure 23 - Effect of inlet oxygen concentrations on the flue gas temperature.

Figure 23 reveals that an increase in the oxygen concentration leads to a slight rise in the flue gas temperature between 21-40%, increasing from 1266°C to 1335 °C. The temperature increase can be explained due to the reduction of the N_2 flow rate that provides a more oxygen-rich environment and a more complete combustion, increasing the energy release.

4.3.4 Flue Gas Emissions

The flue gases monitored were CO , CO_2 , and NO_x . The numerical results for pollutants mass fraction at the outlet are shown in Figures 24, 25 and 26. The values presented in each graph were obtained through the average of the transient values computed in ANSYS Fluent, excluding the initial transient phase and they are detailed in Appendix C.2.

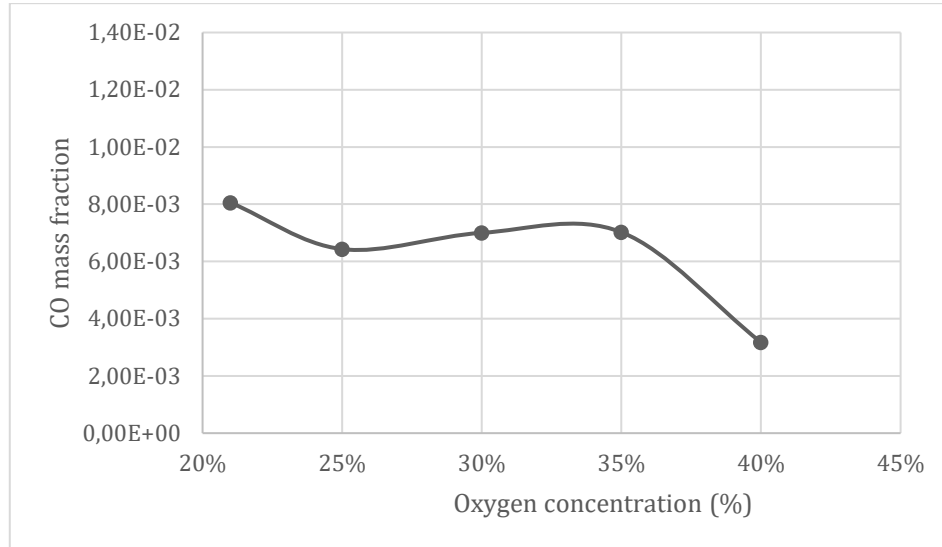


Figure 24 - Effect of inlet oxygen concentration on the CO mass fraction at the outflow stream.

Figure 24 shows high CO concentrations predicted at low percentages of O_2 in the inlet stream. The concentration of this component at the outlet decreases when the inlet stream is oxygenated, which is consistent with the literature, ranging between 3.17×10^{-3} and 8.05×10^{-3} of mass fraction. This trend happens due to the O_2 enrichment in the air stream, leading to a more complete combustion and a reduction of CO in the exit stream.

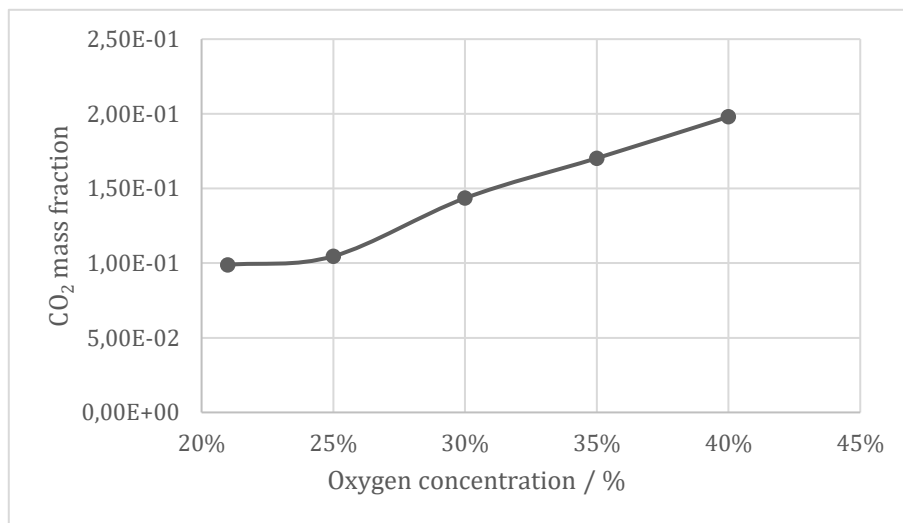


Figure 25 - Effect of inlet oxygen concentration on the CO₂ mass fraction at the outflow stream.

Figure 25 exhibits a consistent trend of increase of CO₂ in the outflow stream with the increase in O_2 concentration at inlet in line with the literature, with an increase in CO₂ mass fraction from 0.099 to 0.198. The presence of CO₂ is expected in any combustion process, and as the

oxygen enrichment rate rises from 21% to 40%, it means a closer approximation to complete combustion, resulting in larger CO_2 concentrations.

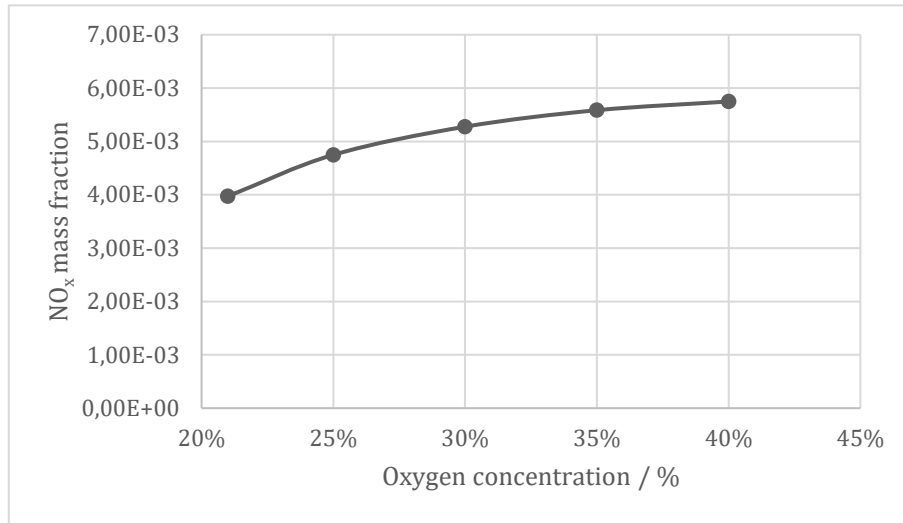


Figure 26 - Effect of inlet oxygen concentration on the NO_x mass fraction at the outflow stream.

The inlet composition has been enriched with oxygen and a reduced amount of nitrogen results in a higher percentage of NO_x released. Figure 26 demonstrates that NO_x emissions increase with increasing inlet oxygen concentration, as temperatures also increase (the thermal-NO mechanism dominates at higher temperatures as stated in De Persis et al. (2013)). The NO_x flue gas concentration rose gradually from 3.97×10^{-3} to 5.75×10^{-3} as O_2 inlet concentration increased from 21% to 40%. However, it can be noticed that the curve flattens above an oxygen content of 30%, indicating the reduction of the influence of O_2 concentration on this pollutant emission, with increments of 5.9% and 2.9% in the last two cases. Thus, the NO_x flow rate at the exit stream was calculated and it shows a slight decrease from baseline case to case 5, between 0.026 kg/s and 0.021 kg/s, respectively. This points out that higher oxygen contents in the air stream can lead to a reduction in flue gas emissions, which is ecologically and economically positive.

5 Conclusion

This dissertation concerned the investigation on the effects of the combustion process when enriching the inlet stream with O_2 , varying its concentration between 21% and 40 %, while reducing N_2 flow rate. The energy availability, temperature and velocity fields, and flue gas emissions were analyzed and discussed.

Turbulent non-premixed natural gas-air combustion in a chamber with a nominal capacity of 410 t_{glass}/day was numerically simulated. A four-step process was developed in ANSYS software, with the execution of the CC geometry, mesh generation, set-up of each model and post-processing results. The CFD simulations were done at transient state, using the $k-\epsilon$ turbulence model and the discrete ordinate method was employed to solve the radiative.

The main results agree with the data available in the literature. The velocity magnitude decrease for enriched O_2 feeds since the inlet mass flow rate is lower for higher O_2 inlet concentrations, affecting the turbulence and leading to a shorter flame. Also, the energy availability for glass melting slightly increase, ranging from 14808 kW to 15179 kW. Since at higher O_2 inlet concentration, the N_2 flow rate decreases, more energy will be available for heating the glass stream instead of the spending energy in heating the inert gas.

For the conditions established, the maximum temperature in the CC increases between 2399°C and 2516°C and the flame became shorter and more intense, explained by the smaller velocities and lower total flow rate at higher O_2 concentrations. The flue gas temperature at the outflow stream increased from 1266°C to 1335°C when the inlet air was enriched with O_2 .

The flue gases monitored were CO, CO_2 , and NO_x . The concentration of CO at the outlet decreased when the inlet stream was oxygenated, ranging between 3.17×10^{-3} and 8.05×10^{-3} of mass fraction. The trending of CO_2 emissions rose from 0.099 to 0.198 because the decrease in the N_2 mass flow rate with the increasing inlet O_2 concentration. The NO_x flue gas concentration increased gradually from 3.97×10^{-3} to 5.75×10^{-3} as O_2 inlet concentration increased from 21% to 40%, showing smaller increments of 5.9% and 2.9% in the last two cases.

To sum up, these results show that higher oxygen contents in the air stream inlet can lead to a reduction in CO emissions, an increase in NO_x and an increase in the energy available to heat the melting glass.

6 Assessment of the Work Done

6.1 Objectives Achieved

The main objective set for this dissertation was to investigate the effects of oxygen enriched combustion in an end port regenerative furnace with different concentrations of oxygen, maintaining the total mass flow rates of O_2 and natural gas through Computational Fluid Dynamics. The variables (pollutant concentration, temperature and velocity fields, the flame length, and the energy availability) computed using ANSYS and the analysis of the data was done successfully, meeting the expected results. The goals set for this dissertation were ambitious and the last objective established was the financial analysis for the different cases. However, due to the delay in processing the simulations, it was not possible to investigate that component, which can be a project to continue in the future.

6.2 Final Assessment

In my opinion, the contribution to emission reduction and energy saving in the company has made me grow in several dimensions, as it is a topic related to one of the most discussed problems of our time. CFD is very attractive from a business point of view and acquiring this type of knowledge can be of great benefit in the future, since I can create a mesh for a specific case, assemble the simulation case and post-process the results obtained. I didn't have the opportunity to properly learn in deeper this software, but with the bases I acquired I hope I can learn more in the future.

This project made me have mixed feelings during its execution, but in this final phase I feel proud for challenging myself to work out of my comfort zone, allowing me to develop my capacities and show my potential.

Finally, a suggestion for a future study is to compare with a technical and financial analysis the heat transfer efficiency for a case with lower O_2 content, with a longer and less intense flame but with heat distributed around the entire glass surface, with the case with a shorter and more intense but locally distributed flame.

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Appendix A Volumetric Flow Rate of Oxidizer

To calculate the O_2 volumetric flow rate at the baseline case, some parameters must be known, such as the fuel volumetric flow rate and the air to gas ratio.

$$Q_{O_2} = 0.21 \times Q_{fuel} \times air/gas\ ratio \quad (22)$$

$$Q_{O_2} = 0.21 \times 34047 \frac{Nm^3}{day} \times \frac{1}{24} \frac{day}{h} \times 13.5 = 4022 \frac{m^3}{h}$$

Thus, the following equation can be used to determine the volume flow of the oxidizer in the various cases of O_2 mole fraction. An example of calculation is shown for baseline case, with 25% of mole fraction of O_2 :

$$Q_y x_{O_2y} = Q_{y-1} x_{O_2y-1} \quad (23)$$

$$Q_y = \frac{19151.57 \frac{m^3}{h} \times 0.21}{0.25} = 16087 \frac{m^3}{h}$$

where, Q corresponds to the volumetric oxidizer flow rate and x_{O_2} to the O_2 mole fraction. The same method was applied to the other cases.

Appendix B Velocity Fields

Velocity vectors for different O_2 mole fractions can be visualized in Figure 27, showing the decreasing of this parameter as O_2 concentration in the inlet stream increases.

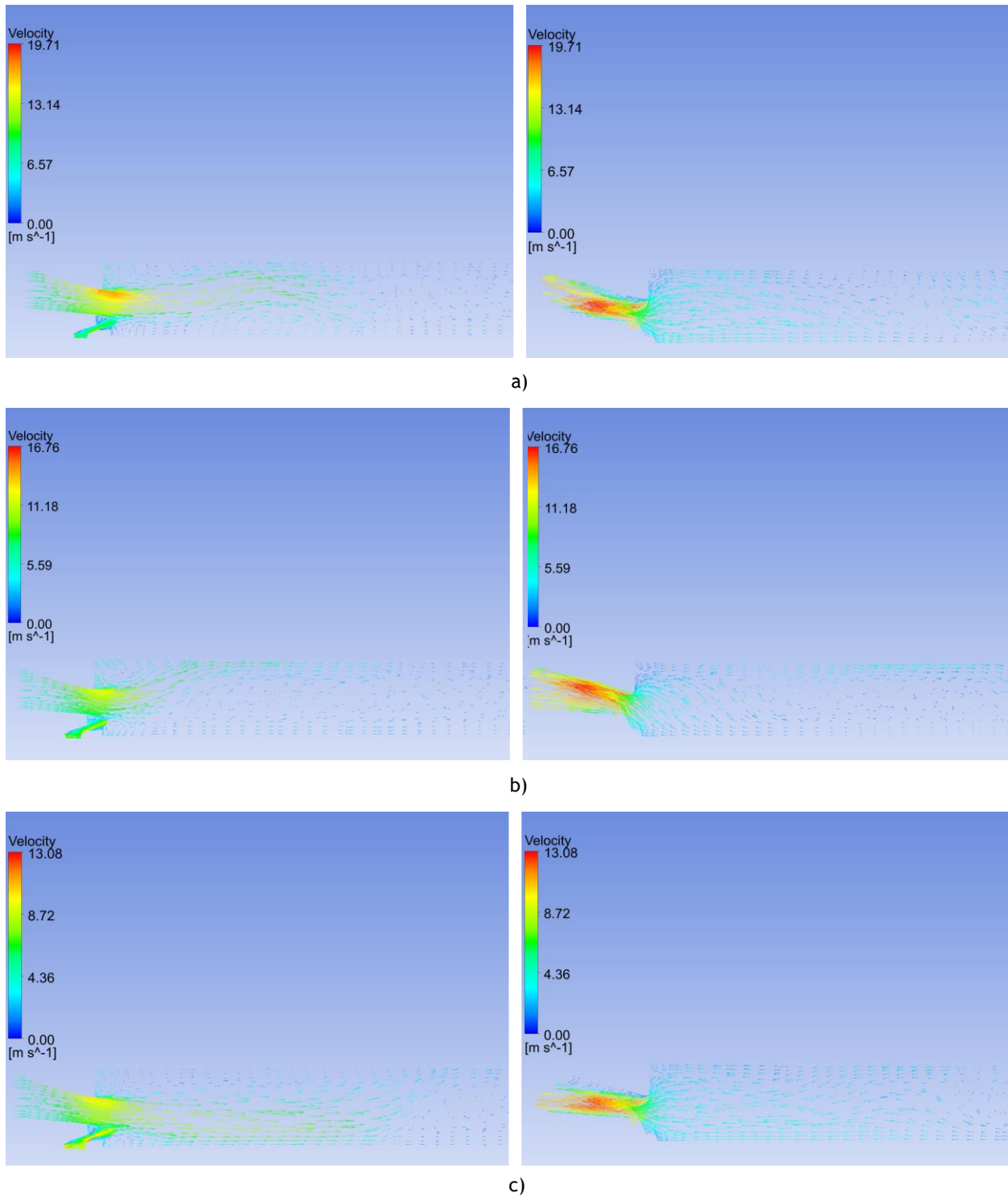


Figure 27 - Inlet and outlet velocity vector fields for different oxygen concentration a) 25%; b) 30%; c) 35%

Appendix C Combustion Variables

C.1 Temperature

Table 7 presents the maximum and outlet temperature of the combustion chamber with the mean, maximum, minimum, and standard deviation of each variable since the behavior of the solution is pseudo-transient.

Table 7 - Maximum and outlet temperatures in each case in °C.

		Baseline	O ₂ enrichment			
		Case 1	Case 2	Case 3	Case 4	Case 5
Temperature (°C)		21%	25%	30%	35%	40%
Maximum	Average	2398.90	2463.89	2492.34	2505.65	2516.16
	Max	2443.56	2494.21	2543.50	2559.35	2559.25
	Min	2360.91	2421.55	2445.66	2462.38	2480.31
	Stand.Dev	10.11	12.86	20.94	16.66	11.17
Outlet	Average	1265.87	1301.01	1309.78	1330.40	1266.16
	Max	1711.56	1796.63	1718.71	1719.37	1683.43
	Min	1036.96	1027.17	1056.01	1102.32	964.29
	Stand.Dev	143.63	186.83	146.72	145.21	219.10

C.2 Pollutants Mass Fraction

Regarding the enrichment of O₂ in the air stream, the mass fraction of pollutants was calculated using the inputs set in ANSYS and through the obtained plots, mean, maximum, minimum, and standard deviation are shown in Table 8.

Table 8 - Mass fraction of pollutants in each case.

Mass Fraction		Baseline	O ₂ enrichment			
		Case 1	Case 2	Case 3	Case 4	Case 5
		21%	25%	30%	35%	40%
CO ₂	Average	9.89×10^{-2}	1.00×10^{-1}	1.05×10^{-1}	1.43×10^{-1}	1.70×10^{-1}
	Max	1.35×10^{-1}	1.23×10^{-1}	1.46×10^{-1}	1.90×10^{-1}	2.16×10^{-1}
	Min	6.52×10^{-2}	6.67×10^{-2}	6.22×10^{-2}	1.14×10^{-1}	1.24×10^{-1}
	Stand.Dev	1.42×10^{-2}	1.32×10^{-2}	1.95×10^{-2}	1.64×10^{-2}	1.83×10^{-2}
CO	Average	8.05×10^{-3}	6.43×10^{-3}	7.00×10^{-3}	7.02×10^{-3}	3.17×10^{-3}
	Max	6.85×10^{-2}	4.43×10^{-2}	5.38×10^{-2}	3.57×10^{-2}	1.23×10^{-2}
	Min	4.15×10^{-6}	3.35×10^{-6}	7.41×10^{-6}	1.43×10^{-5}	1.22×10^{-5}
	Stand.Dev	1.41×10^{-2}	8.56×10^{-2}	1.43×10^{-2}	9.93×10^{-3}	3.42×10^{-3}
NO _x	Average	3.97×10^{-3}	3.94×10^{-3}	4.75×10^{-3}	5.28×10^{-3}	5.59×10^{-3}
	Max	4.99×10^{-3}	5.04×10^{-3}	6.10×10^{-3}	5.94×10^{-3}	6.38×10^{-3}
	Min	3.04×10^{-3}	2.95×10^{-3}	3.84×10^{-3}	4.52×10^{-3}	4.87×10^{-3}
	Stand.Dev	3.23×10^{-4}	3.90×10^{-4}	4.22×10^{-4}	2.64×10^{-4}	3.07×10^{-4}