Aspects Of Mesh Generation For The Burner Optimization Of An Anode Baking Furnace

Internship Report

by

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to obtain the degree of
Master of Science in Chemical engineering,
at the Delft University of Technology.

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Cogito, Ergo Sum
I think, therefore I am

René Descartes

Abstract

Aluchemie produces anodes for the Aluminium industry and is the largest stand-alone anode factory in the world. Anode baking process The anode baking process is one of the crucial steps in the production of anodes for the aluminium industry. It improves the strength, conductivity of the anode and reduces reactivity during electrolysis. Efficient baking involves uniform heat distribution on the surface of the Anode. Hotspots appear close to the burner due to high local temperature gradients. Hotspots lead to an increase in unwanted NO_X emissions. NO_X emissions can be reduced by having an efficient burner design to create a wide temperature distribution and subsequently avoid hotspots. The temperature distribution in the furnace is highly dependent on the flow distribution, combustion and the heat transfer. Accordingly, a model needs to be developed that can model the above-mentioned phenomena and predict the NO_X emissions.

State of the art review shows that there are many mathematical models available for the functioning and operation of ABF. But only a few of the models are tailored to estimate the emissions. Furthermore, these simulations are performed on the geometries with the simplest burner design, even though it is known that the burner configurations, significantly affect the emissions. Therefore, in the current study, a more sophisticated burner design is considered. Due to the complex nature of the burner design aspects of mesh generation are studied in detail and recommendations are made to improve the quality of the mesh.

Acknowledgements

I wish to express my sincere appreciation to my supervisors Domenico Lahaye and Gabrie Meesters. Domenico has the substance of a genius: he is an all-time inspiration. He took it upon himself to push me to think out of the box. Gabrie Meesters lead all the meetings, which helped me to make a better path throughout my Internship. Without their persistent help, the goal of this project would not have been realized. Heartfelt thanks to my PhD supervisor and the pillar of support, Prajakta, who devoted substantial time to have in-depth discussions with me. Her scrutiny and her patience encouraged me to move forward when faced with a road-block.

It's a pleasure to have Guillaume Vergouwen as my company supervisor. I am glad that you gracefully accepted my internship request. I also want to say thanks for the wonderful plant visit at Aluchemie and explaining me practical aspects of plant operation.

I want to recognize the assistance of Frank Heinke from Innovatherm and Franjo Juretic from Creative field provided. Not least of all, I wish to thank my family whose emotional assistance was a milestone in the completion of this project, and all my friends, who helped me stay sane.

Chaitanya Bhatraju
Delft, August 2020

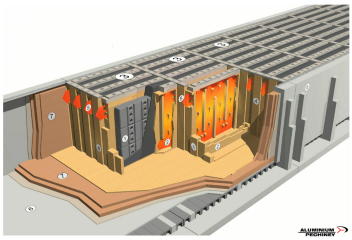
CONTENTS

List of Figures

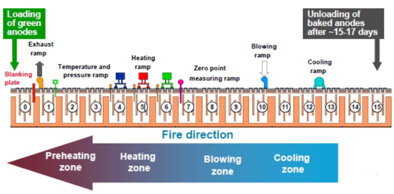
1

INTRODUCTION

The anode baking process is one of the crucial steps in the production of aluminium. Baking improves the strength, conductivity of the anode and reduces reactivity during electrolysis. At Aluchemie, fresh anodes are baked in an open ring furnace, as shown in Figure 1.1a, where anodes are placed inside the furnace pits. The furnace walls provide the heat necessary for baking the anode and also helps in cooling it. The heating and cooling are done by the gases flowing through the walls of the furnace. The location of heat exchange zones is changed sequentially by changing the position of the burner. Thus a single anode, as shown in Figure 1.1b goes through different parts of the process over time. In the preheating zone, the anode is heated using the waste heat from the heating section to release the undesired volatiles. Partially-heated anodes are then heated at high temperatures up to 1100 ^oC to remove all the remaining volatiles[2]. A large amount of necessary heat is generated using burners operating on natural gas. After the heating zone, anodes are cooled in intervals first by blowing cold air and then using external cooling facilities.



(a) Schematics of ABF



(b) Different heat-exchange zones in ABF

Figure 1.1: Overview of Anode Baking Furnace (ABF)[1]

In the heating zone, due to combustion and high temperatures, NO_X emissions are relatively high and is of interest to the present work. NO_X emissions occur when Nitrogen in the air reacts with Oxygen at temperatures greater than 1600 ^{o}C[3] also called as thermal NO_X. Since combustion is an exothermic reaction, the released heat energy can increase the local temperatures above 1600 ^{o}C, generating NO_X emissions. To reduce NO_X emissions it is essential to eliminate local hotspots by efficiently distributing heat within the system. Therefore, efficient baking involves uniform heat distribution on the surface of the anode.

Optimising NO_X emissions requires establishing causal relations between NO_X emissions to the process and design parameters of the anode baking furnace. The cause-effect plots require a detailed understanding of local changes of field variables such as pressure, velocity and temperature. Local changes can be predicted efficiently using the fundamental concepts of Computational Fluid Dynamics (CFD). In the anode baking furnace, the temperature and its distribution are affected by Combustion reaction, Turbulent flow, Heat transfer and Design of the Furnace and the Burner. Modelling of the process in ABF is challenging as all the four phenomena are intimately connected with each other and have to be considered together to predict emissions.

Modelling of Anode Baking Furnace process improved significantly through the years. Early models are relatively simple and are aimed at furnace operation and performance [4, 5]. More sophisticated models are developed later to assist in the design of the furnace [6–8]. Despite the effort, most of the mathematical models lack the ability to predict the carbon and NO_X emissions. Nakate et al. [7] developed a 2D reactive turbulent flow model with radiation to predict NO_X emissions. The results show that the model significantly underestimates the emissions because of its inability to accurately capture the flow and mixing events close to the burner and walls. As a solution, Nakate et al. [7] shifted to a 3D model to better estimate the flow close to the fuel inlet.

1.1. PROBLEM DESCRIPTION

In the Anode Baking Furnace non-premixed combustion of methane and air occurs in the heating zone. The temperature distribution and the distribution of reactants and products are highly dependent on the flow of the gases and on the design of the furnace & burners. Therefore, it is evident that to optimise emissions through modelling and simulations, the first step is to precisely calculate flow field variables close to the walls and capture the mixing events at the end of the burner. There are two main barriers to overcome:

Burner Design The burner configuration can influence the mixing behaviour next to it and consequently have an effect on the size, temperature and location of the flame.[9–11]. These changes to the local process parameters have a direct impact on the emissions observed at the end of the process. Therefore, in the current study, instead of a simple fuel pipe, a more complex burner geometry used by Aluchemie in their day to day operations is considered.

Mesh Generation Nakate et al. [12]. showed that the use of a boundary layer meshes to improve the efficiency of the simulations as well as the accuracy of the solution. An important aspect of the ABF geometry is the varying length scales that differ by at least three orders of magnitude. Burner geometry, among various parts of ABF, has the smallest length scale. It also has the highest sensitivity to the output. This further puts emphasis on having a good quality mesh that can sufficiently resolve the smallest details and is also computationally efficient. Therefore, the current study considers the aspect of mesh generation in detail.

COMSOL Multiphysics® software is used to create the geometry of the Anode Baking Furnace with a complex burner design. COMSOL is selected as it has a well-defined and intuitive interface for integrating a variety of physics and is therefore beneficial to use it in hindsight. For the analysis of mesh generation, an external third-party meshing software, cf-Mesh® is chosen. cf-Mesh creates Cartesian meshes that are suitable for CFD simulations and is interesting to know how it compares with the unstructured meshes from COMSOL.

1.2. Research Questions

Based on the above problem description, the objective of this work is "to investigate the aspects of mesh generation for the burner optimisation of an Anode Baking Furnace" and following research questions are formulated to achieve it:

1. What are the design parameters for optimising the burner geometry?
2. How to quantify a good quality mesh?
3. How to discriminate among various meshes using the quality metrics?

1.3. Report Outline

Chapter 2 discuss the geometry of the burner and explain the choices behind the design parameters. Chapter 3 analyses various mesh quality metrics and aims to develop a meshing philosophy to obtain a good quality mesh. Chapter-4 summarises the report with highlights and future outlook.

2

BURNER DESIGN

The current mathematical models for Anode Baking Furnace focuses on modelling the entire process to anticipate the effect of design or process parameters. In these models, the geometry of the burner is often simplified by considering a fuel pipe with continuous gas injection. This simplification is justified as it reflects the global behaviour of the furnace and also reduces the calculation time[10]. In the current study, the final objective is to predict NO_X emissions. The experimental evidence shows that the burner design has a strong influence on the emission levels. Mahieu and Sedmak [11] showed that just by changing burner configurations, NO_X emissions can be reduced by 20 times. Therefore, a more sophisticated burner design is considered, and in this chapter, the geometry of the burner is described in section 2.1. section 2.2 discusses the heuristic-concepts that lets us choose burner design parameters. The list of burner design parameters and selection among them is done in section 2.3.

2.1. GEOMETRY

The burner design used in the daily operations at Aluchemie is show in Figure 2.1. It consists of a tube with varying diameters in the middle through which fuel is injected. The restriction at the nozzle has an inner diameter (A) of 6.5 mm. The fuel tube is protected by an annular tube with eight holes at the top to induce an airflow for the combustion zone. It has an inner diameter (B) of ≈27 mm. The injection depth (C) of the burner is ≈10 cm.

2.2. DESIGN PHILOSOPHY

The design of the burner is one of the least studied aspects in Anode Baking Furnace despite its effect on NO_X emissions. As a result, the selection of design parameters for burner optimisation studies is not obvious. The current section discusses the heuristics for the *low NO_X emissions - burner design*, to chose the key design parameters that have an impact on the process. Heuristics are developed by analysing research [2, 9–11] as well as the patents for various gas-injecting burners [13–15] that are used in different applications with similar operating temperatures as ABF.

The analysis showed that to reduce NO_X emissions, the design should create a fuel-rich region followed by a fuel-lean region. In the fuel-rich region, high temperatures are created increasing the burner energy efficiency. Due to the lack of availability of Oxygen in the fuel-rich region, NO_X emissions are lower. In the fuel-lean region, the partially burnt fuel can be burned at low temperatures to avoid thermal NO_X formation. The generation of fuel-rich and fuel-lean regions is often achieved by doing staged-air combustion where air/Oxygen is supplied at a different location or time to change the air/fuel ratio. The burner design should also focus on the mixing rate and residence time in both regions. The common observations among various burner designs [13–15] is that the burner should provide:

1. Relatively longer residence time in the fuel-rich regions to burn more oxygen with the fuel
2. Relatively lower mixing rate in fuel-rich region such that the combustion reaction depends on turbulent-mixing than on the reaction rate
3. Higher mixing rates in fuel-lean regions to have a uniform temperature distribution

2.3. DESIGN PARAMETERS

The burner used at Aluchemie creates fuel-rich region using induced airflow from the air inlets and the fuel-lean region is created when the mixture meets the flue gases in the flue-wall. To control the mixing rate and residence time in fuel-rich regions, the following design parameters are considered:

- **Number of air-inlets:** By changing the number of air-inlets the air to fuel ratio in the fuel-rich region can be controlled. Also, the arrangement of air-inlets around the burner can create a swirling flow that can affect the mixing characteristics
- **Nozzle diameter of fuel pipe (A):** SBesson et al. [10] work showed that increasing the nozzle diameter helped in the reduction of thermal NO_X due to having longer residence time and lower mixing rate in the fuel-rich region. The improvement to NO_X emissions is compensated by the increase the CO emissions at the end of the process.

Besson et al. [10] showed that the injection depth has no significant effect on NOx emissions but instead reduce the lifetime of the burner with increasing length. Hence the parameter is not chosen as a design parameter. The design of flue-wall i.e the placement of tie-bricks has an effect on mixing patterns in the fuel-lean region. These design parameters are given as input to COMSOL to create a geometry that changes with the design parameters and therefore can be used in a parametric study.

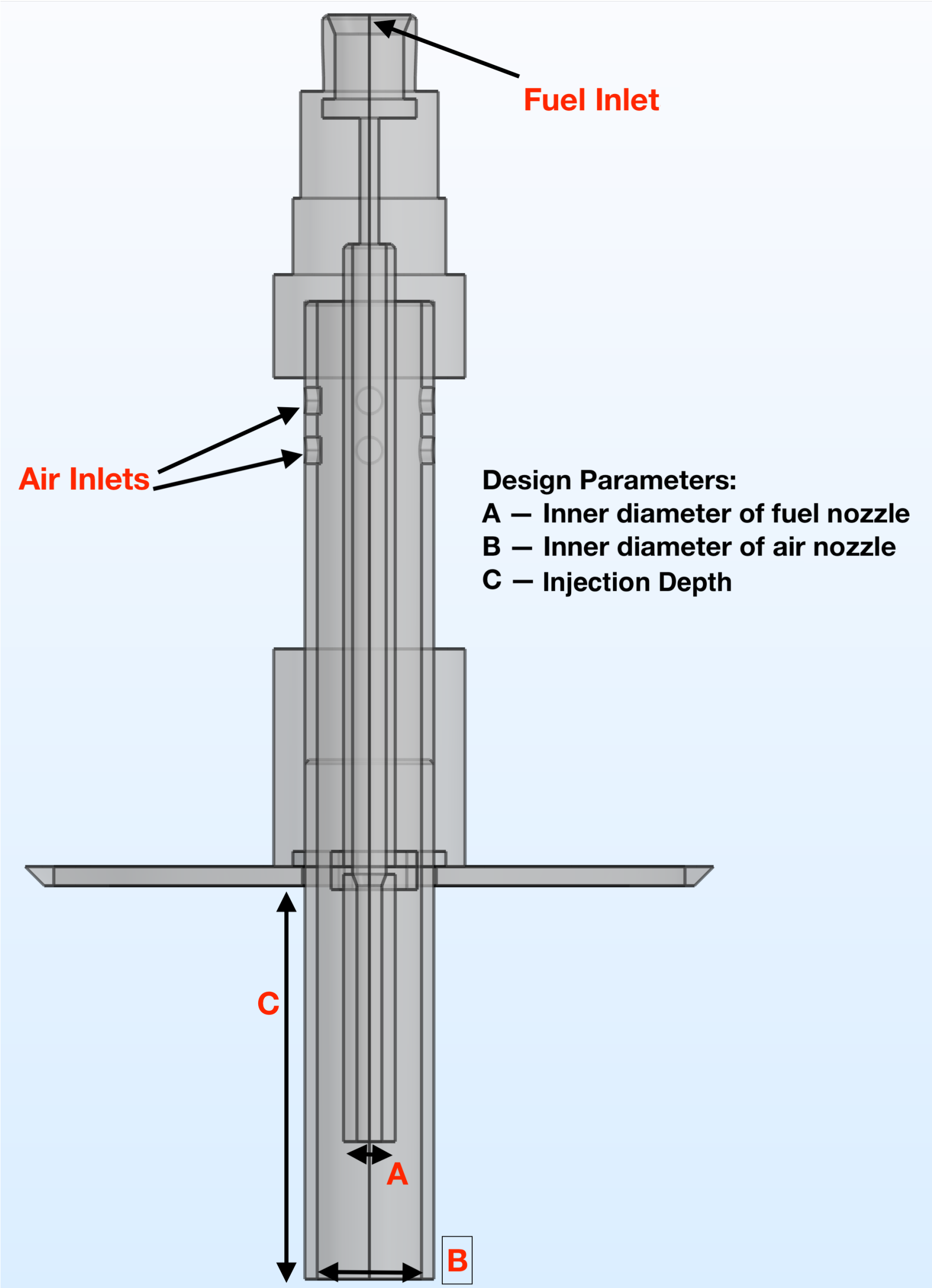


Figure 2.1: 3D Burner geometry labeled with design parameter created using COMSOL CAD Modules®

3

The Art Of Meshing

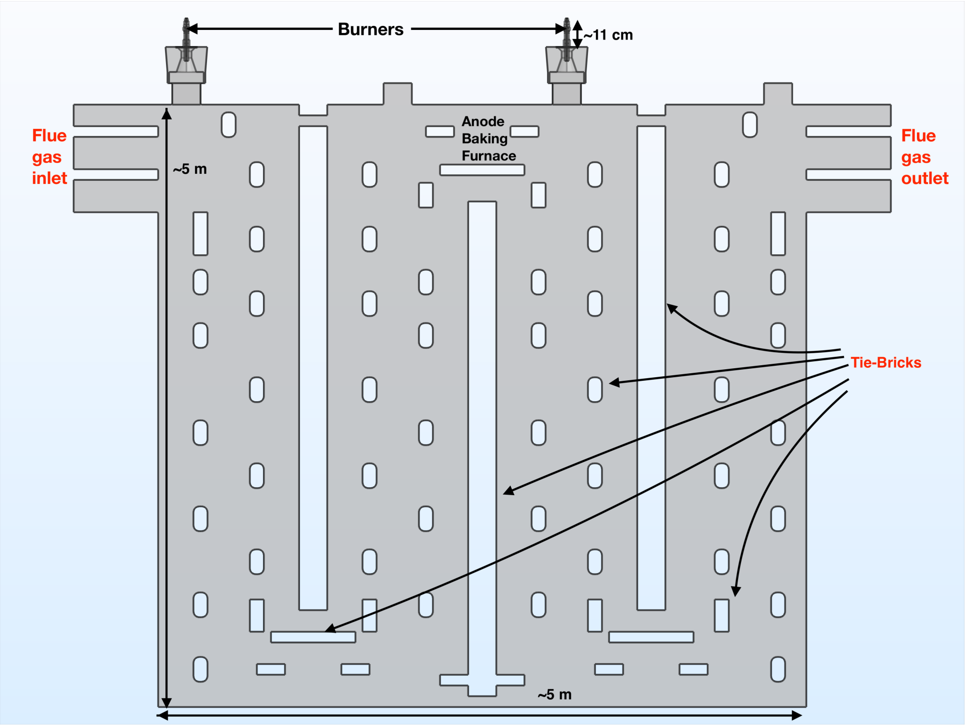


Figure 3.1: ABF with the new burner design and peep hole created using COMSOL CAD Modules®

Mesh generation is a crucial step to get accurate results. In the current study, creating a suitable mesh is a challenge because of the complexity of Anode Baking Furnace geometry. ABF, as shown in Figure 3.1, has components at various length scale ranging from 5m to 5mm. It also has sharp corners and curved surfaces. In the previous chapter, we discussed the effect of burner design and flow on the emissions. And the changes to the design parameters occur at the smallest length scales in ABF. Therefore, a "suitable" mesh for ABF should be sensitive to the small changes in the geometry and contain boundary layers close to the walls and tie bricks.

3

Meshing in COMSOL is not straight-forward, especially for complex geometry. It requires frequent user-input, repetitive analysis and to a certain extent user-intuition. The effort might be justified if the user only needs to generate the mesh once. But for the burner optimisation, a parametric-study with the design variables is necessary and thus need faster mesh generating tools. For that reason, we choose an external third-party tool, cf-Mesh®. cf-Mesh uses the concept of mesh modifiers to generate volume meshes of high quality[16] with minimum user input and computational time. The meshes generated from cf-Mesh are Cartesian meshes that are frequently used for CFD simulations. Cartesian mesh gives more accurate flow results compared to the unstructured or tetrahedral mesh, with the same number of elements[17]. Jeong and Seong [18] showed that the CFD solvers based on FEM depend on mesh quality and size for accurate results. In this chapter, we consider different mesh quality criteria and use them to select the meshes from COMSOL and cf-Mesh.

3.1. MESH QUALITY CRITERIA

Meshes from COMSOL and cf-Mesh can be compared by evaluating them using quality metrics. In this section, we look into the quality metrics that are used in COMSOL and discuss their usefulness in mesh generation. In COMSOL, a mesh is perfect if it is isotropic and has ideal elements such as equilateral triangle, square. Any deviation from ideal element decreases the quality of the mesh and accordingly anisotropic meshes such as boundary layer mesh usually have lower average quality. The deviation from the ideal element is measured using six mesh quality parameters and quality is assessed. The quality of each element is rated between 0 and 1 and the average quality is calculated and the distribution of elements is presented on a histogram. Since the output of this quality assessment is always normalised to 0 and 1, it is a great tool to assess meshes from different platforms. The metrics used for mesh quality are described below[19]:

Skewness Skewness is the default measure in COMSOL and is based on Equi-angular skew. It punishes elements with both large and small angles compared to the ideal element and is calculated according to Equation 3.1. It is important to note that, the skewness definition that COMSOL uses differ from the skewness used in Finite Volume Methods, which is based on the distance between cell centers[17, 20].

$$S = 1 - max\left(\frac{\theta - \theta_e}{180 - \theta_e}, \frac{\theta_e - \theta}{\theta_e}\right) \tag{3.1}$$

where θ is angle over a vertex (2D) or an edge(3D) under consideration and θ_e is corresponding angle of the ideal element and S is the minimum skewness among every vertex(2D) or edge(3D) of an element

Maximum Angle Maximum angle penalises only large angles from the definition of skewness.

Volume verses circumradius Volume verses circumradius is effected by large and small angles as well as the aspect ratio and is calculated as:

$$V_1 = a * \frac{\text{Element volume}}{\text{Volume of circumscribed sphere of the element}} \tag{3.2}$$

where a is a normalising factor to calculate the element quality

Volume verses length Volume verses length is sensitive to aspect ration and is calculated as:

$$V_2 = b * \frac{\text{Element edge length}}{\text{Volume of the element}} \tag{3.3}$$

where b is a normalising factor to calculate the element quality

Condition Number Condition number quality measure is based on the condition number of the transformation matrix between actual and ideal elements.

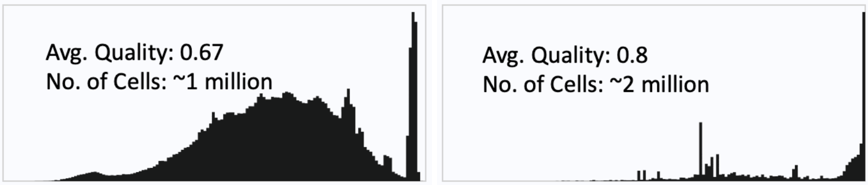
Growth rate Growth rate measures the size of the local element to its neighbors. For a good quality mesh growth rate should be < 20%. The quality based on growth rate is defined as:

$$\frac{min(s_\alpha(E), s_\alpha(E_\alpha))}{max(s_\alpha(E), s_\alpha(E_\alpha))} \tag{3.4}$$

where $s_\alpha(E)$ is size of element E, E_α is the neighboring element in the direction α.

The six quality criteria are dependent on each other and show similar trends for a particular mesh. In the current study, we choose skewness, as it is used by default in COMSOL, to compare the quality of meshes from COMSOL and cf-Mesh. Nakate et al. [12] studied the effect of unstructured mesh and Cartesian mesh, for the Anode Baking Furnace with simple burner geometry (a pipe), on the turbulent flow results. They said, "the disparity in the size and structure of the mesh has a major influence on the differences in the results."[12]. They found that Cartesian mesh is better than the unstructured mesh from COMSOL especially in the region close to the fuel inlet indicating a higher mesh quality for Cartesian Mesh. Using skewness as mesh quality criteria we arrive at the same conclusion for the simplified geometry as shown in Figure 3.2. The figure shows the expected high quality for the Cartesian mesh generated by cf-Mesh [1]. Therefore, mesh quality criteria of COMSOL can be used to assess the meshes generated from the third-party software within COMSOL and can be used to comment on the accuracy of the results i.e a high-quality mesh produces more accurate results.

[1]Enlarged images of the mesh can be found in the Appendix A



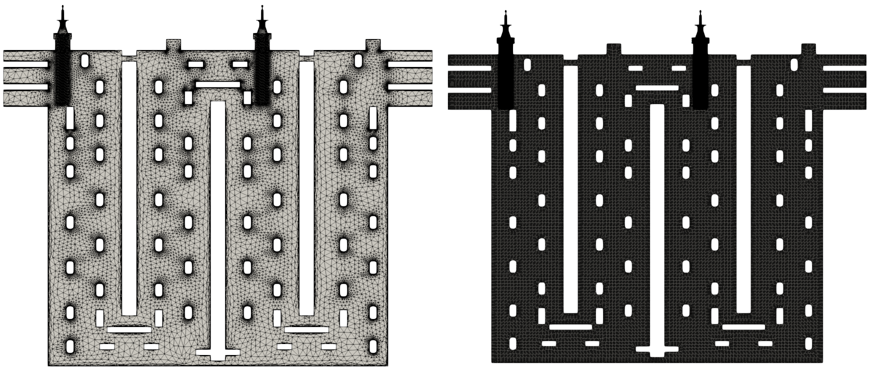
(a) Histograms for the mesh generated using COMSOL (b) Histograms for the mesh generated using cfMesh

Figure 3.2: Histograms for the mesh, of the ABF with simplified burner geometry, based on the skewness mesh quality criteria

3

3.2. ABF WITH COMPLEX BURNER GEOMETRY

The meshes for the ABF with the complex burner geometry are shown in Figure 3.3[2]. And the quality characteristics are shown in Figure 3.4. Figure 3.4a shows the same behaviour as the mesh generated for the simple geometry in COMSOL with low average element quality of 0.67. Whereas the mesh generated in cf-Mesh, as shown in Figure 3.4b has elements of very high quality, but ≈ 0.8% of the elements are of very low quality.

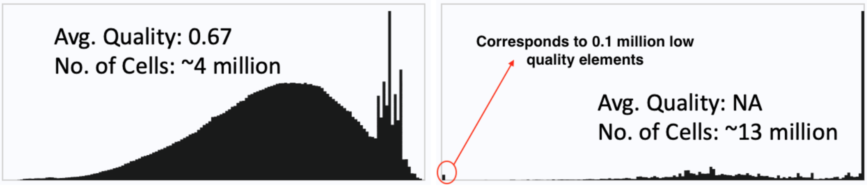


(a) Mesh generated using COMSOL (b) Mesh generated using cf-Mesh

Figure 3.3: Meshes for the ABF with complex burner geometry

Although, there are low-quality elements observed, when imported in COMSOL, no such elements were reported while checking the mesh using check mesh Utility from OpenFOAM®. This is because that cf-Mesh workflow is commonly used for CFD simulations using Finite Volume Methods and the mesher is optimised for FVM. Although low-quality elements can be avoided by refining the regions of low quality, the mesh generated by cf-Mesh already has very fine cells. Therefore, for practical reasons, it is recommended to optimise the mesh generation of cf-Mesh using the skewness criteria of COMSOL. This can help in shifting the low-quality elements into acceptable limits and in the end, provide a mesh with high average quality that is suitable for CFD simulations.

[2]Enlarged images of the mesh can be found in the Appendix A



(a) Histograms for the mesh generated using COMSOL (b) Histograms for the mesh generated using cfMesh

Figure 3.4: Histograms for the mesh, of the ABF with complex burner geometry, based on the skewness mesh quality criteria

Mesh quality plot of the mesh generated using cf-Mesh, as shown in Figure 3.5 and shows that the source of low-quality elements is the burner region, where the number of corners, narrow regions and curved surfaces is high. Therefore, it is recommended to focus on meshing the internal components of the burner separately and combine them later for a better mesh.

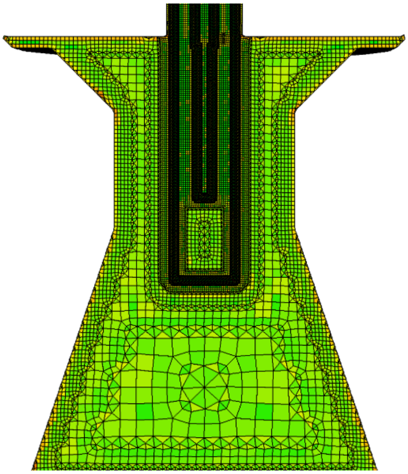


Figure 3.5: Quality plot for "cf-Mesh mesh" generated in COMSOL highlighting the low quality regions Modules. Here the green elements indicate very high quality, yellow indicates average quality and red indicates the worst quality.

4

Conclusion

In the current study, various aspects of pre-processing, for the simulation of Anode Baking Furnace are considered. At first, a geometry with a complex burner geometry was created with the help of COMSOL Multiphysics. In chapter-2, based on the dimensions and literature review on low-emission burners, design parameters are chosen for parametric study. Finally, mesh generation is studied in detail. The deliverables of the work are:

1. Geometry of Anode Baking Furnace with a more sophisticated burner design
2. Design parameters for the burner design
3. A matlab code to create ABF geometry that changes with burner design parameters
4. A mesh of Anode Baking Furnace generated in COMSOL and cf-Mesh
5. Mesh quality criteria - skewness for optimising meshing algorithms in cf-Mesh, and to create a mesh that is optimised for COMSOL Multiphysics.

4.1. Recommendations

For future studies the following recommendations were made:

1. Meshing the burner separately from the flue wall, can give more control over quality of mesh in the burner region
2. Performing some turbulent flow simulations in the generated meshes can help in optimising the element size and quality even further.

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A

Mesh Images

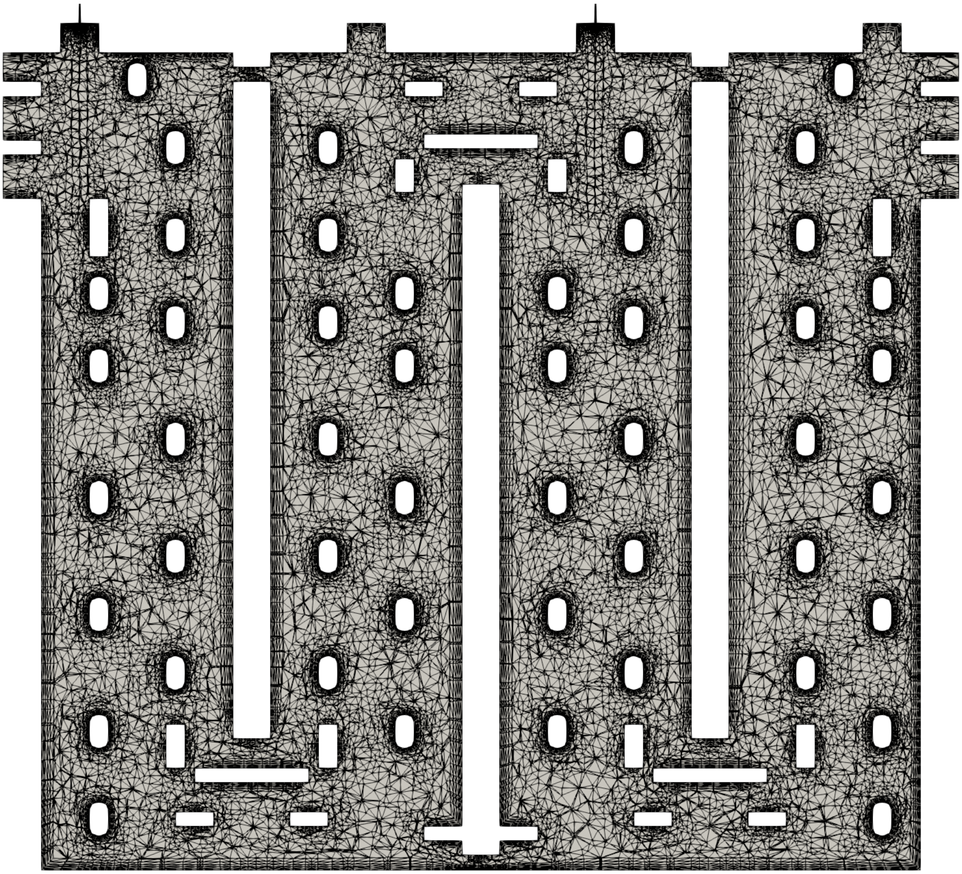

Figure A.1: ABF Mesh with simple Burner design generated in COMSOL

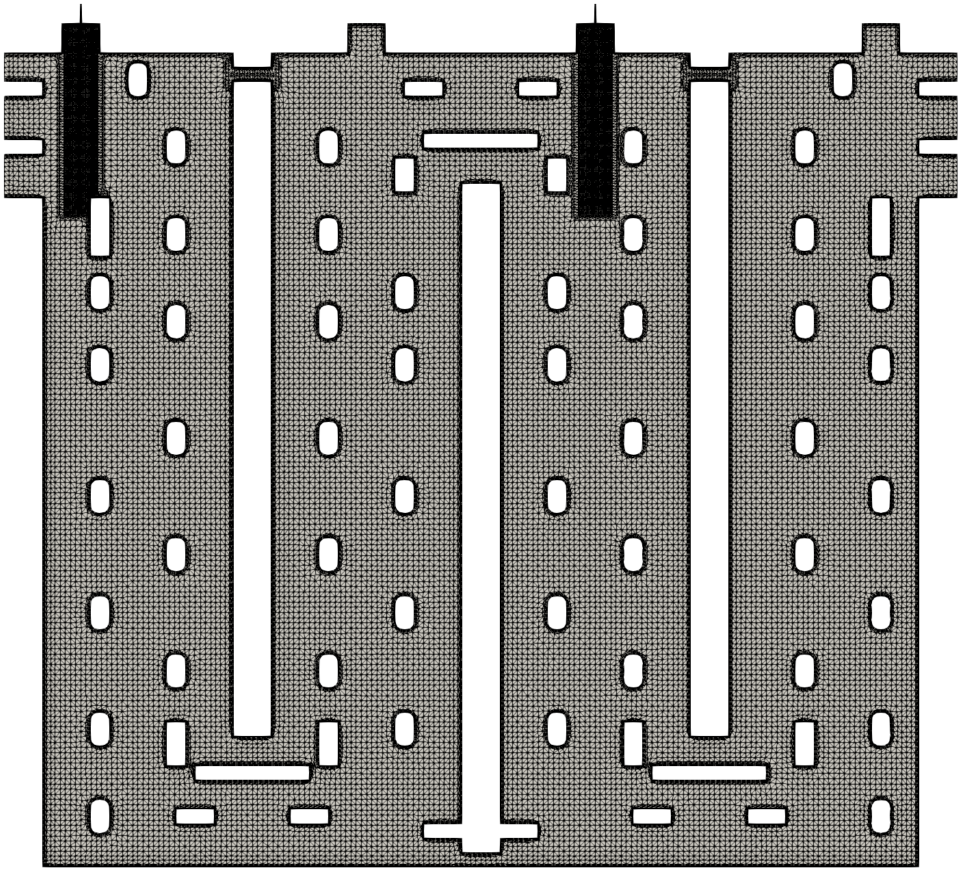

Figure A.2: ABF Mesh with simple Burner design generated in cf-Mesh

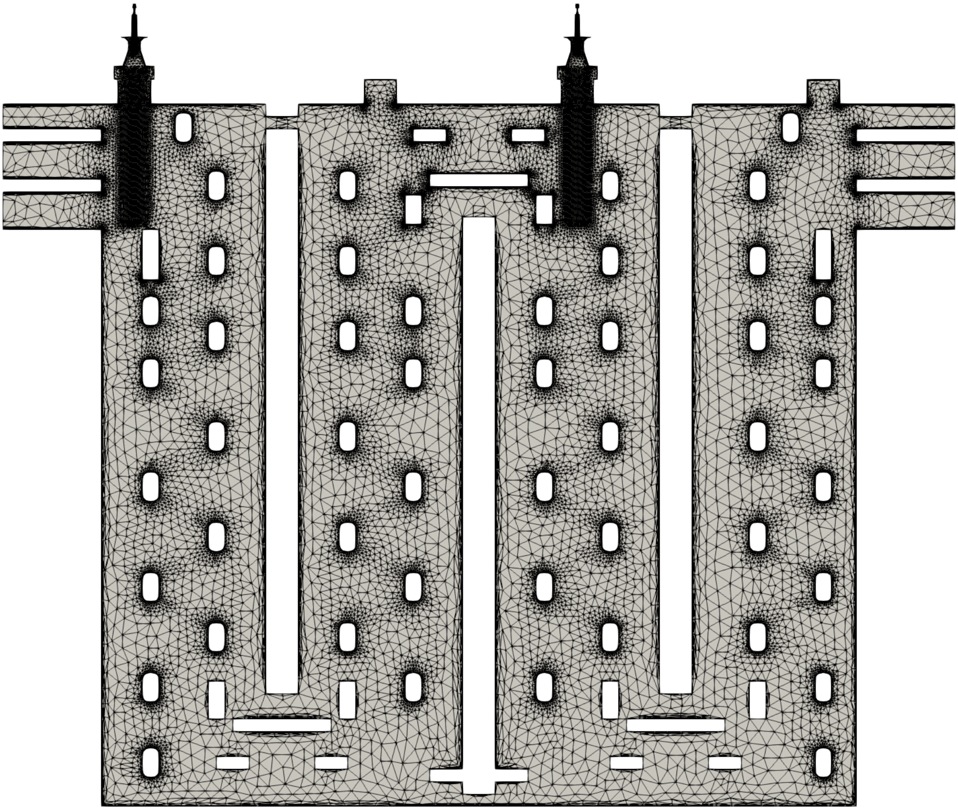

Figure A.3: ABF Mesh with complex Burner design generated in COMSOL

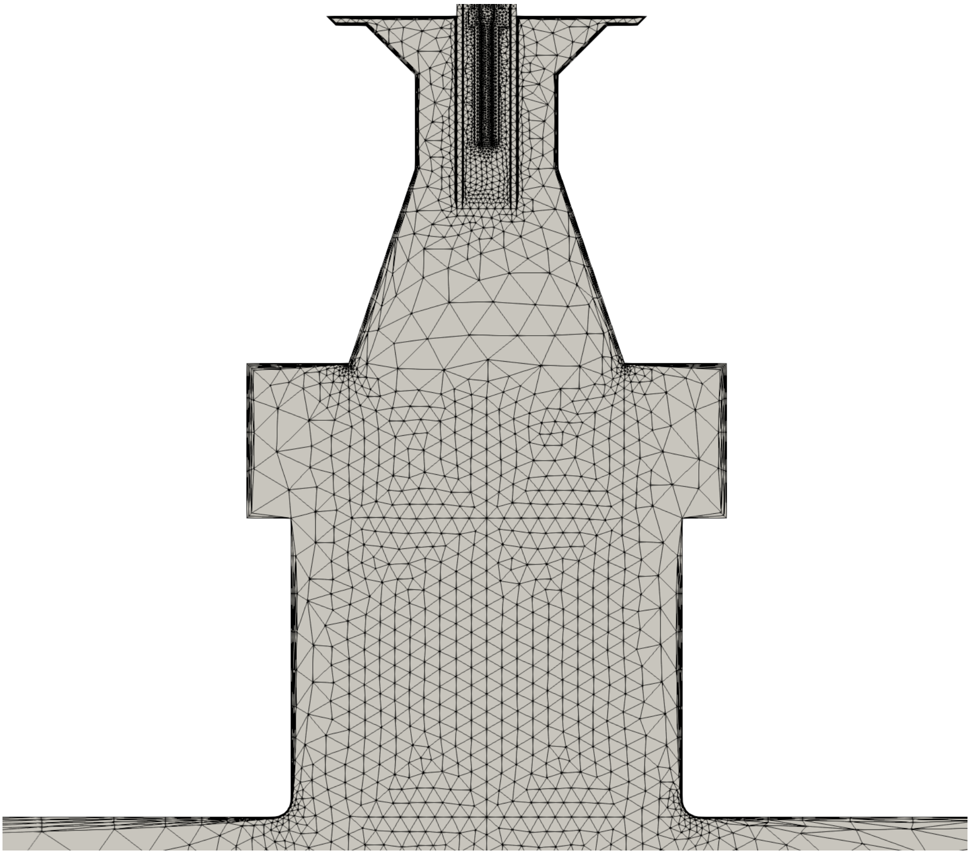

Figure A.4: ABF Mesh with complex Burner design generated in COMSOL, close-up on the burner region

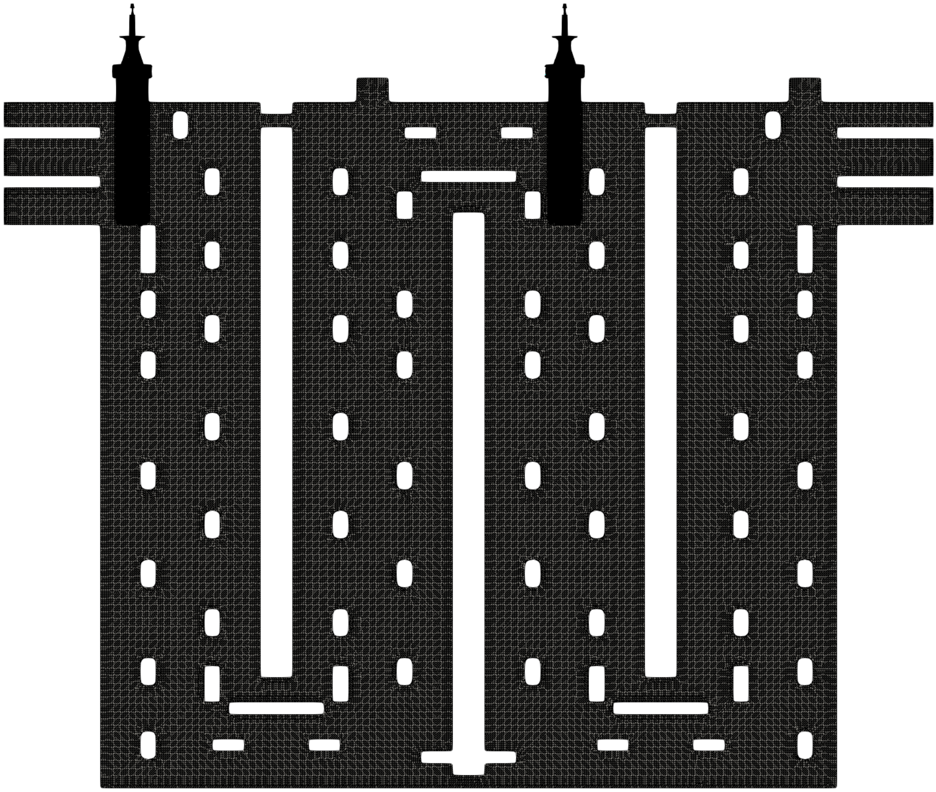

Figure A.5: ABF Mesh with complex Burner design generated in cf-Mesh

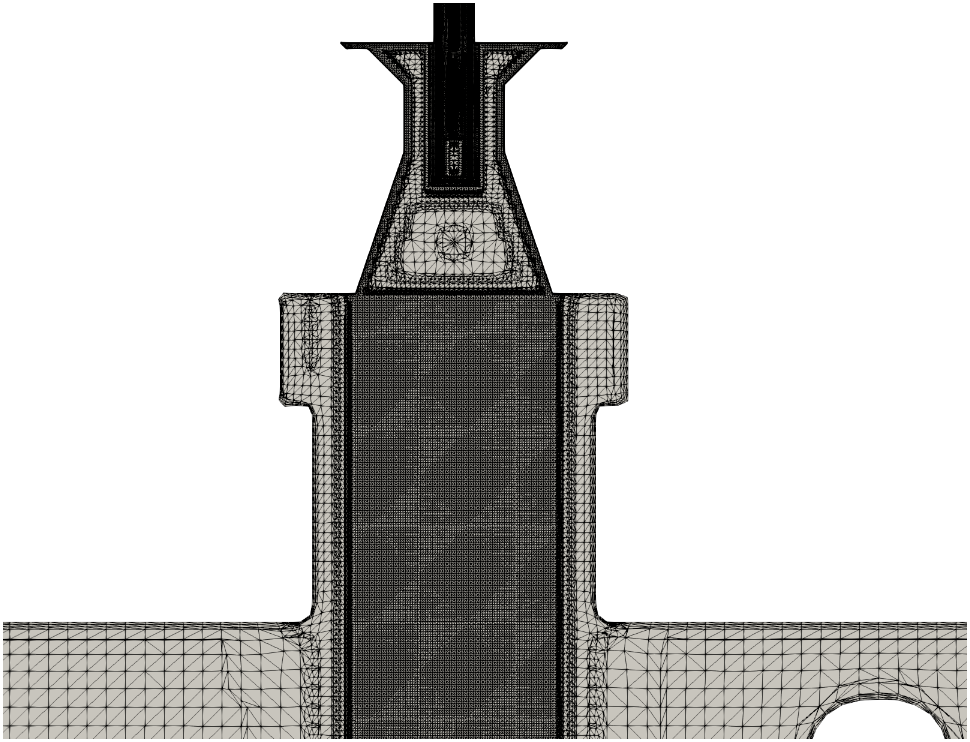

Figure A.6: ABF Mesh with complex Burner design generated in cf-Mesh, close-up on the burner region