A computational analysis of heat transfer in an air-cooled proton exchange membrane fuel cell for unsteady flow conditions and feasibility of heated turbulence grid in subzero conditions.

Master Thesis - Thermal Energy and Process Engineering TEPE4-1000

> Aalborg University Energy Technology



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STUDENT REPORT

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#### Abstract:

Within telecom applications, the aircooled fuel cell, as a backup power system, has recently been gaining popularity. In this study, a CFD analysis has been conducted on the effect of placing a turbulence inducing grid before the cathode inlet of the fuel cell by using three different RANS-based turbulence models, namely RSM, realizable k -  $\epsilon$ , and SST k -  $\omega$ . Moreover, two mesh types were used, specifically conformal unstructured poly hexcore and non conformal structured hexahedral mesh. Additionally, a feasibility study of placing a heated turbulence inducing grid before the cathode in subzero conditions, was conducted. Four different grid dimensions were tested. The results indicate an increase in turbulent intensity when a turbulence inducing grid is placed before the cathode and thus an increase in convective heat transfer. Moreover, a temperature reduction of the solid materials, namely gas diffusion layer and bipolar plate of  $\approx 2.8^{\circ}$ C can be obtained when the grid is placed 2.5mm from the cathode. Results from the heated grid showed preheating the air by 10°C would be feasible, since the grid surface would be  $\approx 236^{\circ}$ C and the power usage would be  $\approx 30\%$  of the total fuel cell power. No remarkable reduction in temperature was found, when a 20 % variation of the inlet velocity was considered. Fuel cell startup time was calculated to be  $\approx 470$  seconds.

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#### Summary

Fuel cells are electrochemical devices that take fuel as input and produce electricity as output. For a PEM fuel cell, the chemical energy stored in hydrogen is converted into electrical energy. The chemical reaction taking place in a PEM fuel cell is given below:

$$2H_2(g) + O_2(g) \rightarrow 2H_2O(l) + 286\frac{kJ}{mol}$$

The chemical process is exothermic, which results in energy being released as seen above. However, due to irreversible factors, such as entropy generation within the process only 237.34 kJ/mol can be converted into electrical energy. This is known as the Gibbs free energy and is the enthalpy of formation differentiated from the irreversible processes occurring in the reaction. The Gibbs free energy limits the theoretical fuel cell potential to 1.23V. Nonetheless due to voltage losses, such as kinetic, ohmic, and concentration losses, the final voltage will often be below 1 V. The remaining energy will be released as heat and, if not handled, will deteriorate the materials of the fuel cell and hence lower its efficiency and limit the produced power density. It is therefore of crucial importance to have a cooling system for the PEM fuel cell. One method that is gaining popularity is using incoming air as a cooling medium. Air-cooled proton exchange membrane fuel cells are often used in applications in the range of a few kW. Some examples are telecom back-up systems, unmanned aeronautical vehicles and student race cars. These fuel cells are very simple in their design, since they do not need a secondary coolant loop. However, due to the low specific heat capacity of air and thus limited cooling, the fuel cell has a relative low power density of around  $0.3-0.4 \text{ A/cm}^2$ .

Previous experimental work has been done on the topic by a research group at Aalborg University. In an attempt to increase the convective air heat transfer inside the cathode channel of the fuel cell, a turbulence inducing grid was placed in front of the cathode. The research showed an increase in the convective heat transfer and additionally a 30% increase in power density(*Shakhshir, Gao, and Berning* 2020).

This thesis includes a numerical investigation of the convective heat transfer inside the fuel cell cathode. For simplicity, only a single fuel cell channel is considered and modeled. In addition to this the thesis also includes a study on the feasibility of having a heated turbulence inducing grid in subzero conditions preheating the incoming air, since these fuel cells are also operated in extremely cold conditions. Two mesh types were considered, namely an unstructured conformal poly hexcore mesh and structured hexahedral mesh. Additionally three different turbulence models were used, namely RSM, realizable k -  $\epsilon$  with an enhanced wall treatment, and k -  $\omega$  SST. The RSM was the main turbulence model investigated, since in a previous study(*Lind*, *Yin*, and *Berning* 2020), the model showed potential promising results. The two other turbulence models acted as comparisons. Both steady state and transient simulations were carried out.

The results obtained from the steady state solutions were three fold. It was shown, that a significant increase in turbulence intensity was achieved when a turbulence inducing grid was placed before the cathode inlet. Moreover, the results showed that as the turbulence inducing grid was placed closer to the cathode inlet, the more turbulence intensity was generated. More specifically, the best results were achieved at a distance of 2.5mm from the cathode inlet at which the temperature could be decreased by  $\approx 2.8^{\circ}$ C. However, the results showed some inconsistencies with the RSM model, with both mesh types, where the highest turbulence was created in the boundary layer close to the wall. These results are nonphysical in nature and can be blamed on the fact that the RSM is a high Reynolds turbulence model and mostly applicable to turbulent core flows. The best results were achieved with the k -  $\omega$  SST in terms of temperature, velocity, and turbulence intensity profiles using the structured hexahedral mesh. Regarding the heated turbulence inducing grid, it was shown to be feasible to some degree. The results showed the best scenario was to preheat the air by 10°C, which resulted in a grid surface temperature of 236°C and  $\approx$  30% fuel cell power usage. Concerning the transient simulations, the result showed a fuel cell start up time of 470 seconds to reach the desired temperature. Additionally, a time dependent sinusoidal velocity profile was used as the inlet boundary condition. Including a 20% pulsating inlet flow, showed no remarkable reduction in temperature of the fuel cell solid materials, when the poly hexcore mesh with RSM was applied.

### Preface

This Master Thesis is written as the final assignment for the Masters Degree in Energy Technology at Aalborg University. The title of the research presented in this report is 'A computational analysis of heat transfer in an air-cooled proton exchange membrane fuel cell for unsteady flow conditions and feasibility of heated turbulence grid in subzero conditions'. The authors would like to express their sincere gratitudes to their supervisors, Torsten Berning and Chungen Yin from Aalborg University for their help and guidance. Their support has been invaluable throughout this master thesis.

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## List of Abbreviations

an	anode
C0 <sub>2</sub>	Carbon Dioxide
са	cathode
CO <sub>3</sub>	Carbonate
е-	Electron
HO <sup>_</sup>	Hidroxide
MEA	Membrane Electrode Assemblies
Nu	Nusselt Number
Pr	Prandtl Number
PTFE	Polytetrafluoroethylene
Re	Reynolds Number
RSM	Reynolds Stress Model
SIMPLE	Semi-Implicit Method for Pressure Linked Equations
AFC	Alkaline Fuel Cell
CFD	Computational Fluid Dynamics
CO	Carbon Monoxide
DC	Direct Current
DNS	Direct Numerical Simulations
EWT	Enhanced Wall Treatment



- FC Fuel Cell
- **FVM** Finite Volume Method
- H<sub>2</sub>O Water
- H<sub>2</sub> Hydrogen
- LES Large Eddy Simulations
- **LTPEM** Low Temperature Polymer Electrolyte Membrane
- MCFC Molten Carbonate Fuel Cell
- PAFC Phosporic Acid Fuel Cell
- **PEMFC/PEM** Proton Exchange Membrane Fuel Cell
- **PEM** Polymer Electrolyte Membrane
- **RANS** Reynolds Average Navier Stokes
- **SOFC** Solid Oxide Fuel Cell

## Nomenclature

Δ	Change in the parameter	_
δ	Kronecker delta ( $\delta_{ij} = 1$ if $i = j$ and $\delta_{ij} = 0$ if $i \neq j$ )	-
Г	Diffusion coefficient	$m^2/s$
μ	Dynamic Viscosity	$kg/m \cdot s$
ω	Specific rate of turbulent kinetic energy dissipation	1/s
Φ	Transport Parameter	_
ρ	Density	$kg/m^3$
τ	Shear Stress	Pa



u	velocity vector - u,v,w	m/s
θ	Angle	0
ζ	Stochiometric coefficient	_
G	Gibbs Free Energy	J
Р	Pressure	Pa
$P_{amb}$	Ambient Pressure	Pa
P <sub>sat</sub>	Saturation Pressure	Pa
Q	Heat Flux	$W/m^2$
9	Charge	C/mol
$R_m$	Universal Gas Constant	$\frac{J}{molK}$
Т	Temperature	°C or K
V	Volume	$m^3$
W	Work	J
W <sub>el</sub>	Work extracted from the cell	W
$x_i$	Mole fraction of species i	_
Ŷ	Dissipation of $k/\omega$	$m^2/s^3$
D	Diffusivity	$m^2/s$
G	Generation of $k/\omega$	$m^2/s^3$
Н	Enthalpy	J
Ι	Current	Α
i	Current density	$\frac{A}{m^2}$
k	Thermal Conductivity	$W/m \cdot K$
n	number of electrons transferred	_



RH	Relative Humidity	%
t	Time	S
U	Mean Velocity	m/s
u	velocity	m/s
Е	Cell Potential	V
k	Turbulent kinetic energy	$m^2/s^2$
S	Source Term	_
S	Entropy	J/K
А	Area	$m^2$
F	Faraday Constant	C/mol



## 1 Introduction

#### 1.1 Basic Principle of a Fuel Cell

A fuel cell is an electrochemical energy converter that converts chemical energy of fuel directly into direct current (DC) electricity. Usually a electricity production process requires various energy conversion stages. However, a fuel cell generates electricity in a single stage. The low cost and simplicity of the fuel cells are some of the characteristics attracting the attention of different industries. In the following pages, fuel cell components will be described. However, for now, it can be seen as a black box model where hydrogen and oxygen, reactants, enter and react in it, and DC electricity, water and waste heat, products, are produced as it can be seen in fig 1.1. The timeline of the fuel cell development has a start in 1842, when William Grove developed the first fuel cell. After this, only with Francis T. Bacon, new work was developed in 1937 and in 1952 a 5kW fuel cell stack was constructed. Fuel cells were used in space programs to generate electricity for life support, guidance and communications(Barbir 2012).



Figure 1.1: Working principle of a fuel cell

There are several types of fuel cells. They are grouped according the type of electrolyte used. The fuel cells can be:

- Alkaline fuel cells, AFCs
- Proton exchange membrane fuel cell, PEMFCs
- Phosphoric acid fuel cells, PAFCs
- Molten carbonate fuel cells, MCFCs
- Solid oxide fuel cells, SOFCs

The differences between these fuel cells besides the electrolyte used are the operating temperature and their reactions. The figure 1.2 outlines the basic principles and electrochemical reactions in various fuel cell types. This project is based on a pro-



Figure 1.2: Different fuel cells, their reactions and operating temperatures (Barbir 2012)

ton exchange membrane. This type of fuel cell is also known as polymer electrolyte membrane. To understand the electrochemistry process it is required a fundamentl knowledge of concepts such as oxidation, reduction, anode and cathode. Oxidation is the process where electrons are removed from a species. Reduction is the process where electrons are added to a species. The anode is the part of the electrode where oxidation takes place. The cathode is the part of the electrode where reduction takes place.

Anode reaction:

$$2H_2 \to 4H^+ + 4e^-$$
 (1.1)

Cathode reaction:

$$O_2 + 4e^- + 4H^+ \to 2H_2O$$
 (1.2)

**Fuel Cell Reaction:** 

$$2H_2 + O_2 \to 2H_2O \tag{1.3}$$



As it was previously mentioned, a fuel cell produces electricity by converting the chemical energy of the fuel. To be possible, the fuel cell must be repeatedly supplied with the fuel and oxidant. This condition will affect the perfomance of the fuel cell. This process is dependent on the operating conditions. After the reactants are transported to the electrodes, the electro-chemical reaction has to occur. The rate of the electro-chemical reaction will influence the current generated. Due to this, the use of catalysts is required to increase the reaction rate and therefore, the efficiency of the process. As equations 1.1 and 1.2 show, ions and electrons are consumed and produced. These ions and electrons need to be transported from the place where they are formed to the place they are consumed to keep the charge balance. The transport process for electrons is easy. However, ions are larger and sizeable than electrons, an electrolyte has to provide a trace for the ions to flow. This process represents a significant resistance loss affecting the performance. As it is demonstrated on the equation 1.3 besides electricity, water and waste heat are products and it is needed to remove them from the fuel cell. In PEMFCs, byproduct water can be a problem if it is not taken into account causing the flooding of the cell.

#### **Cell Potential- Polarization Curve**

As it was previously mentioned, 1.23V is the maximum theoretical fuel cell potential. However, two different situations can be consider and none of them will have this maximum value presented - open circuit and closed circuit. The open circuit, with no current being generated, will have a voltage of, typically, around 1V. Concerning the second situation, closed circuit, current will be generated and because of this, it is expected to be even lower the voltage produced owing to dependent voltage losses. There are three different types of voltages losses such as activation losses, ohmic resistance losses and concentration losses.

With regards to the activation losses they are affected by the kinetics of the reaction. They are the main reason of the voltage drop(*Kaur 2016*). While the current increases , the resistance electrons and ions feel while being transported is required to be taken into account since the voltage will drop linearly in a proportional way . This is the main reason for ohmic losses. Finally the third kind of loss is the concentration losses and they are linked with the consuption rate of the reactants. While the cell is operating the concentration of hydrogen and oxygen were feed on the anode and cathode will decrease. This decrease will be higher or lower depending on the amount of current is being generated(*Barbir 2012*). Mark1020 ACS air cooled fuel cell stack by Ballard Power Systems has a maximum operating current density of  $0.385 A/cm^2$ . It can be seen the differences of the PEMFC when considering its beginning and ending of life time in the figure 1.4 From the polarization curve depicted in the figure 1.4 it is possible to see the maximum values





Figure 1.3: Polarization curve of a fuel cell (Barbir 2012)



**Figure 1.4:** A graph of cell voltage and power density as a function of current density at the end of life

of the current when considering the beginning of the life and the end of the life, 0.385A/cm<sup>2</sup> and 0.25 A/cm<sup>2</sup>. Relatively to the power density at the beginning and end of the life the values presented are 0.224W/cm<sup>2</sup> and 0.13W/cm<sup>2</sup>. Since the power density is linearly dependent of the current density, the aim is to operate at higher currents to have higher power densities. Since the main goal is to increase

the current density, a good cooling system is truly important to have. To increase the cooling effect more effective, a turbulence inducing grid is incorporated in the system before the cathode inlet(*Shakhshir, Gao, and Berning 2020*). As the name suggests, the main goal of putting the grid in that location is to create and induce some turbulence in the fluid.

#### 1.2 Fuel Cell Components

In this section all the components of the fuel cell considered in this project will be presented. Along this project only one of the several channels was analyzed in order to decrease the computational cost. This is possible since the fuel cell channels are arranged with symmetry to constitute the entire fuel cell stack. So, as it can be seen in the figure 1.5 several fuel cell channels will constitute a fuel cell and several fuel cells will constitute the fuel cell stack. This arrangement is done to produce the sufficient amount of electrical potential and power output necessary to the applications mentioned in the section 1.1. From the figure 1.5, besides the



**Figure 1.5:** depicts the fuel cell stack. Additionally, a individual fuel cell and fuel cell channel can be seen. The fuel cell channel is the domain use in the project. (Shahsavari et al. 2012)

anode and the cathode channel, the membrane electrode assemblies (MEA) and the bipolar plate are the two main components. The membrane electrode assembly is the combination of the anode/ membrane/ cathode. Depending on the type of membrane its thickness will vary. There are others components such as catalysts layers which are coupled on each side of the membrane. The most common catalyst



#### 1 Introduction

layer is made of platinum and a high-surface-area carbon. The main function of this catalyst layer is to improve the rate of the needed reactions. To ease the transport of reactants into the catalyst layer and also the transport of the products of the reaction, like water, a gas diffusion layer is needed. A gas diffusion layer is a sheet of carbon paper where the carbon fiber are covered with polytetrafluoroethylene (PTFE). Due to the pores a quick diffusion of the gases is possible. As it was already mentioned, the need to have a stack is on account of small voltages produced by the indivudual MEA. A bipolar plate can be made of metal, carbon or composites and their main functions are increasing the structural strenght of the stack and to supply the electrical conduction between cells. In this project, as a simplification, only the gas diffusion layer regarding the cathode side and the bipolar plate was modelled. All the chemical reactions previously mentioned were not modelled, only the resultant heat flux. The resultant heat flux of the gas diffusion layer will be presented later on this project.



### 2 Fuel Cell Thermodynamics

In this section, the laws of thermodynamics with respect to the fuel cell operations. This has to be done to determine the necessary air flow rate and its velocity to successfully achieve fuel cell operation conditions. In this chapter, calculations to determine the amount of heat generated along the cell operation will also be performed.

#### 2.1 Inlet Streams

As it was mentioned before, the first law of thermodynamics will be applied in PEM fuel cell. However, the molar flow rates will be presented before calculating the ethalpy streams. According to (*Berning and Knudsen Kær 2020*), the incoming molar stream of oxygen is:

$$\dot{n}_{O_{2,in}} = \zeta_{ca} \frac{I}{4F} \tag{2.1}$$

where:

- $\zeta_{ca}$  is the cathode stoichometry flow ratio
- F is Faraday constant

Relatively to the nitrogen, the incoming molar stream is:

$$\dot{n}_{N_{2,in}} = \frac{79}{21} \cdot \dot{n}_{O_{2,in}} = 3.7619 \cdot \zeta_{ca} \frac{I}{4F}$$
(2.2)

An important aspect to have in consideration is the inlet relative humidity,  $RH_{in}$ , since the amount of water vapour is entering the cell depends on it and it is given as:

$$RH_{in} = \frac{p_{H_2O}}{p_{sat}(T)} = x_{H_2O} \frac{p_{amb}}{p_{sat}(T)} = \frac{n_{H_2O,in}}{n_{total,in}} \frac{p_{amb}}{p_{sat}(T)}$$
(2.3)

solving for the molar flow of water,

$$\dot{n}_{H_2O,in} = RH_{in} \cdot \frac{p_{sat}(T)}{p_{amb}} \cdot \dot{n}_{total,in} = RH_{in} \cdot \frac{p_{sat}(T)}{p_{amb}} \cdot (\dot{n}_{H_2O,in} + \dot{n}_{O_2,in} + \dot{n}_{N_2,in})$$
(2.4)

and, finally:

$$\dot{n}_{H_2O,in} = RH_{in} \cdot \left(\frac{p_{sat}(T)}{p_{amb}} - RH_{in}\right)^{-1} \cdot (\dot{n}_{O_2,in} + \dot{n}_{N_2,in})$$
(2.5)

Replacing  $\dot{n}_{O_2,in}$  and  $\dot{n}_{N_2,in}$  with the equations 2.1 and 2.2, respectively, the amount



of water entering the cell is presented as a function of the current and stoichiometry as it is presented below:

$$\dot{n}_{H_2O,in} = RH_{in} \cdot \left(\frac{p_{sat}(T)}{p_{amb}} - RH_{in}\right)^{-1} \cdot 4.7619 \cdot \zeta_{ca} \frac{I}{4F}$$
(2.6)

The saturation pressure  $p_{sat}$  is expressed by Antoine's equation and it is a function of temperature (*Berning and Knudsen Kær* 2020):

$$p_{sat}(T) = D \cdot e^{\left(A - \frac{B}{C+T}\right)}$$
(2.7)

where, A = 8.07131, B = 1730.63, C = 233.426. D is a coefficient to convert the units into Pa, D = 133.233. The saturation pressure, considering an ambient temperature, is 3158 Pa.

Considering the anode side, a specific stoichiometric flow ratio and it is assumed dry hydrogen is entering the cell:

$$\dot{n}_{H_{2,in}} = \zeta_{an} \frac{I}{2F} \tag{2.8}$$

#### 2.2 Outlet Streams

Considering the outlet streams, the molar stream for  $O_2$  and  $N_2$  is given, respectively

$$\dot{n}_{O_{2,out}} = (\zeta_{ca} - 1) \cdot \frac{I}{4F}$$
 (2.9)

$$\dot{n}_{N_{2,out}} = \dot{n}_{N_{2,in}} = 3.7619 \cdot (\zeta_{ca}) \cdot \frac{I}{4F}$$
(2.10)

Considering the global reaction 1.3, the amount of water at the outlet is the sum between the water that entered the cell and the water produced along the reaction. As it was assumed by (*ibid.*), all the water produced leaves at the cathode side resulting in a very low anode side stoichiometric flow ratio. The molar stream of water is given by

$$\dot{n}_{H_2O,out} = \dot{n}_{H_2O,in} + \frac{I}{2F} = RH \cdot \left(\frac{p_{sat}}{p_{amb}} - RH\right)^{-1} \cdot 4.7619 \cdot \zeta_{ca} \cdot \frac{I}{4F} + \frac{I}{2F}$$
(2.11)



#### 2.3 Energy Balance

Regarding the fuel cell and its energy balance, the first law of thermodynamics is applied. Using the principle of energy conservation, the energy balance can be written as (*Barbir 2012*)

$$\sum (H_i)_{in} = W_{el} + \sum (H_i)_{out} + Q$$
(2.12)

where  $W_{el}$  is the work extracted from the cell. Q is equal to zero (Q=0) since the system is assumed to be adiabatic. Since  $W_{el}$  is the electrical work of the fuel cell, there is a relation with the cell voltage and current as it can be seen in the following equation:

$$W_{el} = V_{cell} \cdot I_{cell} \tag{2.13}$$

Accordingly to (*Berning and Knudsen Kær 2020*), assuming an ideal gas behaviour, the enthalpy streams are expressed as:

$$H = \sum \dot{n}_i h_i = \sum \dot{n}_i [\bar{h}_f^0 + (\bar{h} - \bar{h}^0)] = \sum \dot{n}_i [\bar{h}_f^0 + \bar{c}_p (T - T^0)]$$
(2.14)

where  $\overline{h}$  and  $\overline{h}_f^0$  are the molar enthalpy and the enthalpy of formation, respectively. The enthalpy of any species consists of two terms, the enthalpy of formation considering the tempeature as 25°C and pressure of 1 atm and the sensible enthalpy due to the change in temperature. The adiabatic gas outlet temperatures are calculated using the reduced first law of thermodynamics:

$$W = \sum \dot{n}_{i,out} \overline{h}_{i,out} - \sum \dot{n}_{i,in} \overline{h}_{i,in}$$
(2.15)

Using the previous equation and replacing it in the energy balance equation it will be given as (*ibid.*):

$$V_{cell} \cdot I_{cell} = \dot{n}_{O_{2,out}} (h - h^0)_{O_2} + \dot{n}_{N_{2,out}} (h - h^0)_{N_2} + \dot{n}_{H_{2,out}} (h - h^0)_{H_2} + \dot{n}_{H_2O_{out}} (h_f^0 + h - h^0)_{H_2O_{out}} (h_f^0 +$$

Two assumptions were done to simplify the case such as the water results as product of the reaction will be in gas phase and the incoming air will be dry, in other words, there will be no water vapor at the inlet. Since all the molar flow rates presented previously and equation 2.16 are dependent of the cell current, it can be cancelled out as it is presented below. According to (ibid.) the equation will be:



$$\begin{split} V_{cell} &= \frac{1}{4F} \cdot (\zeta_{ca} - 1) \cdot (\overline{h_{O_2}}(T_{out}) - 8682 \frac{kJ}{kmol}) \\ &+ \frac{1}{4F} \cdot 3.762 \cdot \zeta_{ca} \cdot (\overline{h_{N_2}}(T_{out}) - 8669 \frac{kJ}{kmol}) \\ &+ \frac{1}{2F} \cdot (\zeta_{ca} - 1) \cdot (\overline{h_{H_2}}(T_{out}) - 8468 \frac{kJ}{kmol}) \\ &+ \left[ \frac{RH \cdot \frac{p_{sat}(T)}{p_{total}}}{(1 - RH \cdot \frac{p_{sat}(T)}{p_{total}}} \cdot 4.762 \cdot \frac{\zeta_{ca}}{4F} + \frac{1}{2F} \right] \\ &\left( - 241.820 \frac{kJ}{kmole} + \overline{h}_{H_2O}(T_{out}) - 8468 \frac{kJ}{kmol} \right) \end{split}$$

A Matlab script was developed to analyse the variations of the average cell voltage when considering different stoichiometric air flow ratios and also different adiabatic outlet temperature. The stoichiometry flow ratio at the anode is constant and assumed to be 1.1. The operating conditions were defined to be 25°C and 30 % of relative humidity at the inlet of the system. The decrease of voltage depicted in



Figure 2.1: Dependency of the operating voltage when considering different stoichiometric flow ratio and adiabatic outlet temperature

figure 2.1 when considering a specific stoichiometry flow ratio is the result of the production of more waste heat and, consequently, the cathode outlet temperature increases. It can be seen apart from the cell voltage, the ambient air temperature and the relative humidity have an impact on the adiabatic outlet temperature. However, the cathode stoichiometric flow ratio,  $\zeta_{ca}$ , is one of the most important



and key parameter when considering a good performance of the fuel cell.

#### 2.4 Heat of Reaction

The equation 1.3 is equivalent to the hydrogen combustion reaction. The previous process is exothermic which means the system releases energy. According to thermodynamics, the generated heat is the difference between the enthalpy of formation of the products and the enthalpy of formation of the reactants.

$$\Delta H = (hf)_{H_2O} - (hf)_{H_2} - \frac{1}{2}(hf)_{O_2}$$
(2.17)

The enthalpy of formation of liquid water is -286kJ/mol (at 25°C). For elements in their standard state the enthalpy of formation is, by definition, equal to zero. Thus, the enthalpy of the reaction is  $\Delta H = -286kJ/mol$ . The negative sign for enthalpy of the reaction 2.17 illustrates the release of heat. The chemical reaction 2.17 can now be re-written.

$$2H_2 + O_2 \rightarrow 2H_2O + 286kJ/mol$$
 (2.18)

As it was previously mentioned, all the products of the reaction must be carried out by the reactant air.

#### 2.5 Theoretical Electrical Work

The enthalpy of formation previously can be seen as the amount of (thermal) energy the system would release. However, the main driver of the fuel cell is to produce electricity. Since it is not possible to convert all the energy into electricity due to the entropy generated with the process, the amount of electricity produced corresponds to Gibbs free energy. Gibbs free energy is given by the following equation:

$$\Delta G = \Delta H - T \Delta S \tag{2.19}$$

Those irreversible losses in energy conversion are given in a similarly way of the



enthalpy of formation:

$$\Delta S = (sf)_{H_2O} - (sf)_{H_2} - \frac{1}{2}(sf)_{O_2}$$
(2.20)

Considering the reactants and products at ambient pressure and 25°C, the values of *hf* and *sf* can be found at thermodynamic tables. Regarding the thermodynamic tables,  $(sf)_{H_2O} = 0.069 \frac{kJ}{mol*K}$ ,  $(sf)_{H_2} = 0.131 \frac{kJ}{mol*K}$  and  $(sf)_{O_2} = 0.205 \frac{kJ}{mol*K}$ . Substituting these values into the equation 2.20, the entropy difference between products and reactants is  $\Delta S = -0.165 \frac{kJ}{mol*K}$ . At 25°C, Gibbs free energy turns out to be  $\Delta G = 237.34 \frac{kJ}{mol}$ .

#### 2.6 Theoretical Fuel Cell Potential

Commonly, electrical work is the product of charge and potential:

$$W_{el} = qE \tag{2.21}$$

where the charge, q, transferred in a fuel cell reaction per mole of hydrogen is determined by 2.22

$$q = nF \tag{2.22}$$

where, *n* is the number of electrons per molecule of  $H_2$  and *F* is the Faraday constant, *F* = 96485*C*/*mol*. Linking the eq.2.21 and eq.2.22, the fuel cell electrical work is given by eq.2.23

$$W_{el} = nFE \tag{2.23}$$

Since the Gibbs free energy is the maximum electrical work in a fuel cell reaction, the following assumption can be done to determine the theoretical fuel cell potential.

$$-\Delta G = nFE \Rightarrow E = \frac{-\Delta G}{nF} = \frac{237340 \frac{J}{mol}}{2*96485 \frac{C}{mol}} = 1.23V$$
(2.24)

With regards to the equation 2.24 and its final result, the actual voltage while operating will be always lower due to inevitable losses.



#### 2.7 Inlet Channel Velocity

In the section "Inlet Channel Velocity", the calculations presented were done to know the velocity at the inlet of the channel. As it was mentioned on the previous sections, the flow rate of the air inside the cathode is one of the most important parameters. So as to achieve the inlet velocity at the cathode, the mass flow rate in duct equation needs to be rearranged:

$$u = \frac{\dot{m}}{\rho \cdot A_{channel}} \tag{2.25}$$

where, the cross sectional area of the channel is represented by  $A_{channel}$ . One of the previous assumptions was the ideal gas behaviour. Therefore, from the ideal gas equation 2.26, and accordingly to (*Barbir 2012*) density is defined as:

$$\rho = \frac{M_{air} \cdot P}{R \cdot T} \tag{2.26}$$

The variables of the previous equation are the molar mass of ai,  $M_{air}$ , pressure, P, and the ideal gas constant, R. Expressing the mass flow rate of the air by the following expression:

$$\dot{m}_{air} = \frac{1}{x_{O_{2,in}}} \cdot M_{o_2}$$
(2.27)

where the molar fraction of  $O_2$  at the inlet is represented by  $x_{O_{2,in}}$ . In the presence of a certain relative humidity, the inlet molar fraction of the water vapor,  $x_{H_2O_{in}}$ , needs to be taken into account. The molar fraction water of the water vapor is given by the ratio of the saturation pressure and the total pressure as it can be seen on the equation 2.28:

$$x_{H_2O_{,in}} = \frac{p_{sat}}{p_{in}}$$
(2.28)

Usually, 79:21 is the ratio between nitrogen,  $N_2$ , and oxygen,  $O_2$ . With this consideration it is possible to calculate the inlet oxygen fraction as it can be seen below:

$$x_{O_{2,in}} = \frac{1 - x_{H_2O_{,in}}}{1 + \frac{79}{21}}$$
(2.29)

Accordingly to (*ibid.*), the oxygen mass is given by the equations 2.30 and 2.31:

$$\dot{m}_{O_2} = \zeta \frac{I}{4 \cdot F} \cdot M_{o_2} \tag{2.30}$$

$$\dot{m}_{O_2} = \zeta \frac{i}{4 \cdot F} \cdot M_{o_2} \cdot A_{MEA} \tag{2.31}$$

Since, the current is the product of the current density and the active area of the fuel cell itself, the equation 2.31 becomes valid. Returning to the starting point, equation 2.25 and, substituting with all the previous demonstrations the velocity at the inlet in now given by:

$$u_{in} = \zeta \frac{I}{4 \cdot F} \cdot A_{MEA} \cdot \frac{1}{x_{O_{2,in}}} \frac{R \cdot T_{in,ca}}{P_{in}} \frac{1}{A_{channel}}$$
(2.32)

The velocity value calculated above with the equation 2.32 is the velocity at the inlet of the cathode. However, the cross-sectional area of the channel that is set before the fuel cell is bigger than the cross-sectional area of the cathode. With this said, a ratio between areas and velocities as to be considered to know the free stream velocity. The assumption of  $\rho$  is constant needs to be considered.

$$b_1 u_{in} A_{ca} = \rho_2 u_{ch} A_{ch}$$
$$u_{in} A_{ca} = u_{ch} A_{ch}$$
$$\frac{u_{in}}{u_{ch}} = \frac{A_{ch}}{A_{ca}}$$
$$u_{ch} = u_{in} \frac{A_{ch}}{A_{ca}}$$

l

#### 2.8 Heat flux of the Gas Diffusion Layer

In this report some assumptions were done. A constant heat flux regarding the gas diffusion layer is one of them. According to(Barbir 2012), the heat generated when considering a fuel cell stack with reactants such as hydrogen and oxygen and by-product of water vapor is given by:

$$\dot{Q} = (1.254V - E_{cell})I \cdot N_{cells}$$
(2.33)

The value 1.254 is the electrolyzer voltage and the  $E_{cell}$  is the cell voltage,  $N_{cells}$  is the number of cells in the stack and I is the current. In this project only one cell is modelled so, the equation 2.34 as to change to:

$$\dot{Q} = (1.254V - E_{cell})i$$
 (2.34)

where, i is the current density and its units is  $A/m^2$ . This current density and cell voltage are dependent and this can be related to all the voltage losses of the fuel cell stack. According to the Mark1020 ACS<sup>TM</sup> fuel cell polarization curve a high current density of 0.385 A/cm<sup>2</sup> should be used. Regarding the previous



dependency, the cell voltage considered will be 0.582V. So, finally, the heat flux can be calculated as it can be seen below:

$$\dot{Q} = (1.254V - 0.582V) \cdot 0.385A/cm^2 = 2587W/m^2$$
 (2.35)

Parameter	Value	Units
Pressure at the inlet	101325	Pa
Temperature at the inlet	293.15	K
Current density	3850	A/m <sup>2</sup>
Cross sec. area of the cathode	$6.82 \times 10^{-6}$	$m^2$
GDL surface area	$3.78 \times 10^{-4}$	$m^2$
Faraday Constant	96485.33	C/mol
Ideal Gas Constant	8.314472	$J/(K \cdot mol)$
Oxygen Mole Fraction	0.21	-
Stoichiometry air flow ratio	50	-

Table 2.1: Parameters used on the first calculation



## **3** Turbulence Inducing Grid

In general turbulence grids are considered to be an essential part in fluid flow problems, where the aim is to either produce or reduce turbulence. Furthermore turbulence grid are also often used when large scale velocity and pressure nonuniformities are desired to become more uniformal(*Roach 1987*). Here the turbulence inducing grids used will be described and shown. Different geometries were used regarding the grid, since the thesis focus was dual, namely to investigate the feasibility of placing a heated turbulence grid in front of an air-cooled fuel cell stack in subzero conditions and furthermore to do an analysis of heat transfer for unsteady flow conditions using a Reynolds Stress turbulence model. Furthermore, in order to minimize the cell count in the computational domain, a symmetry plane was created.





**Figure 3.1:** shows the grid geometry where 6 holes are used in order to generate turbulence as the air passes through the grid

**Figure 3.2:** exhibits the grid geometry where 24 holes are used to generate turbulence as the incoming air passes through the grid

Figures 3.1 and 3.2 show the front view of the grid geometries along with the according measurements. Worth noting is that for the analysis of heat transfer for the unsteady conditions the grid with 6 holes and a depth of 1 mm was used, while for the heated grid simulations, 4 different geometries were used in order to investigate the heated turbulence inducing grid feasibility. The four different geometries are given in table 3.1. Worth noticing is also that the solid volume of the grid is included, since this parameter is an essential part when investigating the grid surface temperature.





**Figure 3.3:** shows the grid geometries with 6 holes and along with different depths

**Figure 3.4:** similarly shows the grid geometries with the two depths for the 24 hole grids

Turbulence Grid	Number of Holes	Depth	Solid Volume
Α	6	1 <i>mm</i>	$4.935 \ mm^3$
В	6	2 <i>mm</i>	9.870 mm <sup>3</sup>
С	24	1 <i>mm</i>	$6.855 \ mm^3$
D	24	2 <i>mm</i>	13.710 <i>mm</i> <sup>3</sup>

 Table 3.1: Grid Dimensions Used For Heat Grid Simulations

#### 3.1 Heated Turbulence Grid in Subzero Conditions

For the steady state simulations concerning the feasibility of a heated grid, four different grid dimensions were used. The turbulence grids are shown in figures 3.1 through 3.4. The total solid volume of the grid for the different dimensions is given in table 3.1.

In order to have a basic understanding of the range of these temperatures associated with the heated grids, it is important to start of with an analytical approach before proceeding to the steady-state simulations.



#### 3.1.1 Rough Estimation of Grid Temperatures

In this particular case, air is being forced to move through the turbulence grid by an external mechanism in order to generate turbulence. This is therefore a case considering convective heat transfer and moreover the rate of the convective heat transfer is expressed by Newton's law of cooling given in equation 3.1

$$Q_{conv} = h \cdot A \cdot (T_s - T_{\infty}) \tag{3.1}$$

where  $Q_{conv}$  is total power, *h* is the convective heat transfer coefficient, *A* is the wetted area,  $T_s$  is the average surface temperature of the turbulence inducing grid, and  $T_{\infty}$  is air average temperature before and after the grid.

To determine the convective heat transfer coefficient h, three dimensionless numbers are needed. These are the Reynolds number, Prandtl number, and finally the Nusselt number (Bergman et al. 2011). Dimensionless numbers are very essential, since they are often a ratio between two physical quantities and give a good overview of the behaviour of a system.

$$Re = \frac{\text{Inertia Forces}}{\text{Viscous Forces}} = \frac{\rho \cdot V \cdot L}{\mu}$$
(3.2)

where  $\rho$  is the density of air, *V* is the air velocity and *L* is the grid length, and  $\mu$  is the absolute viscosity

$$Pr = \frac{\text{Viscous Diffusion Rate}}{\text{Thermal Diffusion Rate}} = \frac{\mu \cdot C_p}{\lambda}$$
(3.3)

where  $C_p$  is the specific heat of air and  $\lambda$  is thermal conductivity of air

$$Nu = \frac{\text{Convective Heat Transfer}}{\text{Conductive Heat Transfer}} = \frac{h \cdot L}{\lambda}$$
(3.4)

To calculate the convective heat transfer coefficient h, an empirical correlation for the averaged Nusselt number for forced convection is given in equation 3.5

$$Nu = 0.664 \cdot Re^{0.5} \cdot Pr^{1/3} \tag{3.5}$$

This empirical correlation for the Nusselt number is for a flat plate, considering laminar flow and a Prandtl number higher than 0.6 since it is not possible to determine a correlation for an average Nusselt number for a customised turbulence inducing grid.

With regards to the previous equations a rough analytical estimation was calculated. Some assumptions were done such as:

- $T_{\infty}$  will be the average temperature between the inlet and outlet of the control volume;
- Prandtl number, Pr, is 0.70;
- The conductivity, k, is  $0.02476 \frac{W}{m \cdot K}$
- The ambient temperature is -20 °C
- The temperature of the fluid after the grid is 5 °C

The Reynolds number regarding the velocity and the length of the grid is given by:

$$Re = \frac{U_{\infty}L}{\nu} = \frac{0.8 \cdot 1 \times 10^{-3}}{1.470 \times 10^{-5}} = 54.42$$
(3.6)

In respect of the previous empirical correlation presented, the Nusselt number is:

$$Nu = 0.664 \cdot Re^{0.5} \cdot Pr^{1/3} = 0.664 \cdot 54.42^{0.5} \cdot 0.70^{1/3} = 4.37 \tag{3.7}$$

Considering equation 3.5 and solving for the convective heat transfer coefficient, the following equation is obtained:

$$h = \frac{Nu \cdot k}{L} = \frac{4.37 \times 0.02476}{1 \times 10^{-3}} = 108.2 \frac{W}{m^2 K}$$
(3.8)

Finally, and using the Newton's Law of cooling, equation 3.1, having  $Q_{conv} = 0.2115W$  was calculated using air velocity, specific heat capacity, and change in temperature. This can be seen in the MATLAB code given in appendix A. This value was found solving for  $T_s$ , the surface temperature of the grid is 1947.2 °C. This results gives a good indication of the range of temperature expected in the heated turbulence inducing grid.
# 4 Problem Statement

The objective of this thesis is to delve into and examine the effect a turbulence inducing grid has on the convective heat transfer inside of a cathode flow channel in a fuel cell channel. Moreover, this investigation will be done with special emphasis on the Reynolds Stress Model(RSM), since previous studies have suggested that the model gives good predictions regarding the topic at hand. Additionally, a comparison between other turbulence models, realizable k- $\epsilon$  and k- $\omega$  SST, and structured and unstructured grids will be performed. Furthermore the thesis will investigate whether it is feasible to heat up the incoming air by a heated turbulence inducing grid in subzero conditions. The modelling and simulations will be done by the use of CFD package ANSYS 2020 R2 student version. The aim of the project is to answer the following problem statement :

Does the turbulence inducing grid before the cathode give an enhancement to the convective heat transfer inside the cathode channel in unsteady flow conditions and moreover is it feasible to have heated turbulence inducing grid to preheat the incoming air in subzero conditions.

These additional research questions will likewise be answered:

- 1. Will a pulsating inlet flow increase the convective heat transfer inside the cathode.
- 2. How much heat input is required for the turbulence inducing grid to preheat the incoming air.
- 3. Is the current grid dimension feasible to preheat incoming air, or should additional grid dimension be implemented.



#### 4.1 Previous Work

#### **Experimental Work**

Previous experimental work has been done on the topic by a research group at Aalborg University(*Shakhshir, Gao, and Berning 2020*). Their experimental work took a starting point from a previous numerical study where it was found that the reason for the limited performance in an air-cooled PEM fuel cell was due to the limited heat transfer. The air stream coming in to the cathode channel, which simultaneously served as a coolant, was limited and thus the proposed idea was to place a turbulence inducing grid before the inlet cathode channel to induce turbulence and hence increase the convective heat transfer inside the cathode. The fuel cell used in the experimental work was a Ballard Mark 1020 ACS stack and multiple turbulence grids varying in pore size, thickness, rib width, angle of pores, and the distance to cathode inlet were tested. With the experiments, the research group concluded that the most important parameter related to increasing the convective heat transfer, and thus the performance, was the distance between the grid and cathode inlet. Moreover, the best results were achieved having a distance between the grid and cathode below 5 mm.



**Figure 4.1:** Shows the polarization curve for the Ballard Power System Mark 1020 ACS<sup>TM</sup> with and without the turbulence inducing grid(*Shakhshir*, *Gao*, and *Berning* 2020)

Observing figure 4.1, it is clear that the power density and fuel cell voltage have increased by up to 20% and 30% respectively. This greatly increases the performance and efficiency of the fuel cell, since the enhanced convective heat transfer aids in cooling of fuel cell.



### **Numerical Studies**

Two previous numerical studies have been conducted on this topic. Both studies were conducted as parts of master thesis at Aalborg University. The first numerical study was conducted by two graduates which tried to replicate the performance increase of the fuel cell by using an available CFD package at the time(*Pløger et al. 2018*). However, their results indicated only a small temperature decrease of the PEM fuel cell when the turbulence inducing grid was implied before the cathode(< 1K). There were some assumptions made regarding constant density and heat capacity of air. One other factor which could contribute to these results could have been the mesh quality. Inadequate mesh quality would result in inaccurate captures of the flow structures inside the cathode.

The other numerical simulation was conducted some time after the first and this numerical study tried to correct some of the small inaccuracies in the first study to aim for a better replication of the experimental work(*Lind*, *Yin*, and *Berning* 2020).



Figure 4.2: Mesh changes from the first numerical study to the latter Lind, Yin, and Berning 2020

The results of the latter numerical study also indicated a temperature decrease of the fuel cell when the turbulence inducing grid was placed before the cathode(3.5K). The reason for this decrease could be due to the mesh changes and re-



finement and moreover since the simulation was done under transient conditions. For the transient simulation the Large Eddy Simulations(LES) was used. However limited by the computational time/resources, the LES was performed based on a coarse mesh of only 60,000 cells, which may not be sufficient to resolve the energy-containing, large, anisotropic eddies. As a result, the reliability of the LES results could be compromised. An agreement was made to try to redo the numerical study using a refined mesh and the comprehensive Reynolds Stress Model for the transient simulation. This thesis includes this numerical study.



# 5 Computational Fluid Dynamics

This section will cover the theory behind the CFD simulations and additionally justify the choice of turbulence model in the simulations. Moreover the section will also give an overview of the pre-processing by describing the computational domain, mesh, boundary conditions, and Physics models and solution methods used in the project.

The Navier - Stokes equations can be written as

$$\frac{\partial(\rho u)}{\partial t} + u \cdot \nabla(\rho u) = f \tag{5.1}$$

and equation 5.1 can be further simplified by relating the conservation of mass and product rule and thus gives

$$\frac{\partial(\rho u)}{\partial t} + \nabla \cdot (\rho u u) = f \tag{5.2}$$

The Navier - Stokes equations express that the rate of change of momentum of a fluid(liquid or gas) finite volume is determined by the external forces acting on the fluid volume.

Three of the most typical forces regarding the external forces acting on the fluid volume are pressure, viscosity and gravity. The full Navier - Stokes equation is given in equation 5.3

$$\underbrace{\frac{\partial(\rho u)}{\partial t}}_{\text{Unsteady Term}} + \underbrace{\nabla \cdot (\rho u u)}_{\text{Convective Term}} = \underbrace{-\nabla p}_{\text{Pressure}} + \underbrace{\nabla \cdot \tau}_{\text{Shear Stress}} + \underbrace{\rho g}_{\text{Gravity}}$$
(5.3)

Besides solving the Navier - Stokes equations, other equations may need to be solved for the related applications. These other equations could be regarding energy, temperature, concentration, turbulence and so on. All of these equations follow a similar template which will be described below.



### 5.1 General Transport Equation

Let  $\phi$  be a general variable introduced to represent a scalar quantity, a general transport equation can be written as:

$$\underbrace{\frac{\partial(\rho\phi)}{\partial t}}_{\text{Unsteady Term}} + \underbrace{\nabla \cdot (\rho u\phi)}_{\text{Convective Term}} = \underbrace{\nabla \cdot (\Gamma_{\phi} \nabla \phi)}_{\text{Diffusive Term}} + \underbrace{S_{\phi}}_{\text{Heat Source}}$$
(5.4)

The governing equations, which will be described in the next section, all follow the template of the general transport equation. The discretization of the governing equations with respect to time and space will be done in accordance to the Finite Volume Method(FVM)(Versteeg and Malalasekera 2007).

### 5.2 Governing Equations

The assumptions made in the numerical study were as follows:

- Incompressible flow, since the air velocity is below Mach 0.3.
- An Eulerian framework is used over a Lagrangian, since the domain only consists of one fluid phase.
- Viscosity is accounted for.
- Gravity forces cared for.

#### **Incompressible Navier Stokes equations**

As mentioned in the previous section, the in compressible Navier Stokes equation given in equation 5.3 describes the fluid flow and will be solved numerically. In addition to equation 5.3 the continuity equation will be solved, due to the fact that when a fluid is moving, it mus move in such a way that mass is conserved.

$$\frac{\partial \rho}{\partial t} \nabla \cdot (\rho u) = 0 \tag{5.5}$$

#### **Incompressible Reynolds Averaged Navier Stokes equations**

In the Reynolds Average Navier Stokes(RANS) equations, the idea of a Reynolds decomposition comes into play. The Reynolds decomposition consist of decomposing the instantaneous values into a mean and fluctuation term given in equation 5.6

$$u = U + u' \tag{5.6}$$

where  $\bar{u}$  and u' are the mean and fluctuation velocities respectively. A general expression for all variables, such as pressure, velocity, and concentration can be given

$$\phi = \Phi + \phi' \tag{5.7}$$

Substituting equation 5.6 into equation 5.3 and 5.5 and taking the time average and expanding gives the RANS expression

$$\underbrace{\frac{\partial(\rho U_i)}{\partial t}}_{\text{Unsteady Term}} + \underbrace{\frac{\partial\rho U_i U_j}{\partial x_j}}_{\text{Convective Term}} = \underbrace{-\frac{\partial p}{\partial x_i}}_{\text{Pressure}} + \underbrace{\frac{\partial}{\partial x_j} \left(\mu \frac{\partial U_i}{\partial x_j}\right)}_{\text{Shear Stress}} + \underbrace{\frac{\partial(-\rho u'_i u'_j)}{\partial x_j}}_{\text{Revnolds Stress}}$$
(5.8)

These Reynolds stresses appear, due to fluctuating velocity field, since the Navier Stokes equations are nonlinear in nature(Versteeg and Malalasekera 2007). To get an equation having only mean velocity and pressure, the Reynolds stresses need to be modelled or computed with a turbulence model. The following section will cover the turbulence model used.

#### **Energy equation**

Moreover, since the task contains heat transfer within a fuel channel, the energy equation also needs to be applied and numerically solved.

$$\underbrace{\frac{\partial(\rho c_p T)}{\partial t}}_{\text{Unsteady Term}} + \underbrace{\nabla \cdot (\rho c_p u T)}_{\text{Convective Term}} = \underbrace{\nabla \cdot \left(\left(k + \frac{c_p \mu_t}{Pr_t}\right) \nabla T\right)}_{\text{Diffusive Term}} + \underbrace{S}_{\text{Heat Source}}$$
(5.9)

where T is the air temperature,  $c_p$  is the specific heat capacity, and k is the thermal conductivity of air.

### 5.3 Turbulence Model

Different simulations methods exist when turbulence is the subject at hand. Among these are Direct Numerical Simulations(DNS) and Large Eddy Simulations(LES). However, the sole focus in the thesis will be on RANS-based turbulence models. There are different turbulence models available to close the RANS equations. They can be separated into three main parts

• Linear eddy viscosity models



- Nonlinear eddy viscosity models
- Reynolds stress model (RSM)

where the first two classes are based on the concept of the eddy viscosity approach and the other is a direct computation of the individual components of the Reynolds stresses. Nonlinear eddy viscosity models will not be considered in the thesis. The eddy viscosity or the Boussinesq approach was first proposed in 1877, by a french scientist called Joseph Valentin Boussinesq. Boussinesq suggested to related the turbulent stresses to the mean flow and thus close the equations. He implemented an analogy method between viscous stresses and Reynolds Stresses and thus introduced the concept of an eddy viscosity. However, this eddy viscosity, contrary to the molecular viscosity, is not a physical fluid characteristic, but a function of local flow conditions in the system(Versteeg and Malalasekera 2007).

$$\underbrace{\tau_{ij} = \tau_{ji} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)}_{\text{Viscous stresses}} \xrightarrow{\text{Analogy Method}}_{\text{Boussinesq(1877)}} \underbrace{-\rho \overline{u'_i u'_j} = \mu_t \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right)}_{\text{Reynolds Stresses}} (5.10)$$

By implementing the eddy viscosity approach given in equation 5.10 the task is to solve for the eddy viscosity. By doing this, the RANS equations will be closed and thus gives a time average solution to the Navier Stokes equations. In addition to this, all eddy viscosity models are isotropic.

#### Standard k - $\epsilon$ Model

It is a two equation high-Re model, where two additional transport equations for turbulent kinetic energy, k and the dissipation rate  $\epsilon$  respectively, are solved to calculate the eddy viscosity,  $\mu_t$ . It is robust and has reasonable accuracy for a wide selection of turbulence flows, however one disadvantage is its insensitivity to adverse pressure gradient for example seen in the wake of a high angle wing or step wall where the flow separates at a step. Since it is a high-Re model, a modification needs to be applied in order to resolve the near-wall region. For it to correctly capture the viscous sublayer behaviour enhanced wall treatment(EWT) is needed(ANSYS 2009).

### Realizable k - $\epsilon$ Model

The realizable k -  $\epsilon$  model differs from the standard k -  $\epsilon$  in two ways. The first is a new formulation for the eddy viscosity. Instead of having the model constant  $C_u$  constant, it now varies with the mean velocity field. The second differentiation from the standard is a new transport equation for the dissipation rate  $\epsilon$  which has



been derived from mean-square vorticity fluctuation. The realizable k -  $\epsilon$  more accurately predicts adverse pressure gradients, flow separation and recirculations (ANSYS 2009).

### Standard k - $\omega$ Model

In a similiar way to the k-  $\epsilon$  model the k -  $\omega$  models solves two additionally transport equations, namely for the turbulent kinetic energy k and the  $\omega$  the specific dissipation rate. The k -  $\omega$  model is applicable in the near-wall region, since it is designed to predict correct behaviour in the boundary layer close to the wall. Therefore no modification is needed. However, it is highly sensitive to free stream boundary condition values of k and  $\omega$  (ANSYS 2009).

### SST k - $\omega$ Model

The SST k -  $\omega$  model is a blended turbulence model, where it explores the advantages of both standard k -  $\epsilon$  and the standard k -  $\omega$ . The inner layers i.e. viscous sublayer, buffer layer, and log-law layer are based on the standard k -  $\omega$  predicting correct behaviour near the wall and in the outer layer it is converted to the standard k -  $\epsilon$  and is therefore applicable to high Reynolds flows aswell(ANSYS 2009).

### **Reynolds Stress Model(RSM)**

The Reynolds Stress Model is a very comprehensive turbulence model. The RSM does not rely on the eddy-viscosity approach like the turbulence models previously described. Instead the model closes the RANS equations by directly solving the Reynolds Stresses. By doing this direct procedure, seven additional transport equations arise and are solved. The RSM model is a high Re model and, similarly to the k -  $\epsilon$  models, needs near wall treatment in order to capture effects close to the wall. Even though the RSM is more complex than the other models, the results are not always superior, when considering different classes of flow. RSM is known to have accurate predictions when taking into account complex flows such as high swirling flows in combustors, cyclone flows, rotating flow passages, and streamline curvature(ANSYS 2009).

#### **Choice of Turbulence Model**

As it was previously mentioned, one part of the project aim was to see whether the turbulence inducing grid would increase the convective heat transfer inside the cathode channel using the RSM model for unsteady flow conditions. Results from previous studies(Lind, Yin, and Berning 2020) showed potential promising results with the RSM model, which ignited the curiosity to investigate if the RSM model



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would indeed give better convective heat transfer results. Two other turbulence models, namely realizable k -  $\epsilon$  and SST k -  $\omega$  were chosen as comparisons to the RSM model.



# 5.4 Computational Domain

Previously, it was presented the most common configuration of a fuel cell. In this chapter an overview of the computational domain used during this project is presented. The objective of setting a turbulence inducing grid before the cathode inlet is to increase the heat transfer rate between the fuel cell components and the fluid along the cell which will release more heat to the fuel cell outside.

In this report a bipolar plate (light grey), a gas diffusion layer (dark grey) and a grid are modelled as the solid cells while the remain parts of the domain are considered as fluid cells of the domain.The figure 5.1 illustrates the computational domain used in this report: There were three main distances when considering the



Figure 5.1: Computational domain used along this report

grid and the cathode inlet, 2.5mm, 5mm and 10mm. However, in figure 5.1 only the first distance is represented. The following figures, figures 5.2 and 5.3, illustrate the front view and the isometric perspective of the bipolar plate. The bipolar plate is important considering the structural support and it supplies the electrical conduction between the different cells. The fluid is housed inside of the bipolar plate and therefore the bipolar plate is also impermeable to gases.





Figure 5.2: Bipolar plate dimensions



Figure 5.3: Length of Bipolar Plate



The figures 5.4 and 5.5 elucidate how the gas diffusion layer is modelled and all its dimensions. As it was mentioned on the section 1.2, the gas diffusion layer has a porous surface (porosity varies between 70% to 80% according to (Barbir 2012) to provide a passage for the reactant gases and it also connects the catalyst layer and the bipolar plate electrically.



Figure 5.4: Length of the Gas diffusion layer



Figure 5.5: Front View of the Gas diffusion layer

Bipolar Plate			
Property	Value	Units	
Density	1970	kg/m <sup>3</sup>	
Specific Heat	720	$J/(kg \cdot K)$	
Thermal Conductivity	20.5	W/(mK)	
Surface Roughness	0	m	

Table 5.1: Bipolar properties used for simulations (Barbir 2012)



Gas Diffusion Layer			
Property	Value	Units	
Density	450	kg/m <sup>3</sup>	
Specific Heat	900	$J/(kg \cdot K)$	
Thermal Conductivity	1.7	W/(mK)	
Surface Roughness	$1 \times 10^{-6}$	m	

**Table 5.2:** Gas diffusion layer properties used for simulations *Toray Carbon Fiber Paper*

### Symmetry Plane

With regards to the geometry presented on figure 5.1, it can easily be noticed the existence of a symmetry when considering a YZ plane. This symmetry plane allows to minimize the number of cells required in the computational domain reducing the time and cost of all the simulations performed along this thesis.



Figure 5.6: Symmetry plane



### 5.5 Mesh

The domain discretization is an absolutely essential part of the process when considering a computational fluid dynamic simulation. The requirement to transform the geometry into numbers is the basis of the discretization process. The spatial



Figure 5.7: The process of meshing before the processing part

discretization is needed to substitute the real space by a finite number of points in that same space - a mesh. Due to the importance of this process to achieve high accuracy on the final solution, the mesh generation can be one of the major time consuming while considering CFD simulations. There are several types and in this project only two different types will be consider which are particularly structured mesh and unstructured mesh. Other types of mesh can be generated such as hybrid meshes or adaptive meshes. A structured mesh is defined by the regular connectivity and characterized by the use of quadrilateral elements hexahedra elements in 2D and 3D, respectively. The adjacent cells have the same disposition and, consequently, are predictable. In other words, the cells can be address and represented by the double indices *i*,*j* or triple indices (*i*,*j*,*k*). A general approach is given by the figure 5.8, where it can be seen how a structured mesh can be created:



Figure 5.8: The index of the nodes regarding 2D and 3D structured meshes (Tu, Yeoh, and Liu 2013)

To have accurate results when considering computational fluid dynamics simulations, the meshing is one of the most fundamental parts to achieve them as it was already mentioned before. Several parameters are used to evaluate and characterize the type and quality of the mesh used such as orthogonal quality, cell skewness and the aspect ratio. With regards to the orthogonal quality, its value will be be-



tween zero and one, where zero will characterize the worst cell while the best cells will assume values close to one. The second parameter, cell skewness, is characterized by the comparison of the actual cell shape and the equilateral cell format. This means a skewness of zero represents a equilateral cell while a skewness of one is a corrupted cell. An atrocious skewness will affect the accuracy and the convergence of the simulation. Last but not least, the stretching of a cell, aspect ratio, is also an important parameter to have in consideration. This is a key factor when analyzing gradients where high aspect ratios should be avoid. A detailed description of all the parameters described can be found at the end of this report on the Appendix C.

### **Orthogonal Quality**

Orthogonal quality is the parameter responsible for evaluating the angles between the neighbour edges or faces of the mesh and comparing it to a optimal angle. The figure 5.9 illustrates the orthogonality concept in cells.



Figure 5.9: Angles between neighbour faces

### Skewness

As it was mentioned before, skewness is one of the major parameters to have into account in order to achieve a good converged solution. This is important because if the cell has a considerable skewness it will be harder to have a final solution since the face fluxes which are normal to the common face of the cells, if these vectors are not normal to the face other variables will have inaccurate values which can and will lead to a divergence.

$$Skewness = max\left(\frac{\theta_{max} - \theta_e}{180^\circ - \theta_e}, \frac{\theta_e - \theta_{min}}{\theta_e}\right)$$
(5.11)



where,  $\theta_e$  is the equiangular face/cell and it depends on the cell element considered. The maximum value skewness should be below 0.95.



Figure 5.10: A non-skewed cell and a skewed cell

### **Aspect Ratio**

The last parameter mentioned is the aspect ratio. This characteristic evaluates the stretching of a cell.



**Figure 5.11:** 2D where the aspect ratio is measured by  $AR=\delta x/\delta y$  or where is the ratio of circumscribed circle/ inscribed circle

**Figure 5.12:** 3D where the aspect ratio is measured by AR=A/B



### Non - Conformal Structured Mesh

A non-conformal structured mesh will be one of the two different types of mesh used in this report. This non-conformal mesh is heavily inspired by a previous study(Lind, Yin, and Berning 2020). The goal of this approach is to compare results when using different spatial discretizations in order to realize if the final profiles of certain properties would differ or present similar results. The comparison of the two mesh types is presented, hereafter a clear idea about the model uncertainty can be assumed. The simplicity of the geometry and the free stream velocity direction are three good parameters to support the use of a structured mesh.

#### **Conformal Polyhexcore Mesh**

Although the simplicity of the geometry and regularity of the computational domain, an unstructured mesh was one of the spatial discretization type chosen due to its fast generation. This was an important factor since previous studies had already used a structured mesh and also a transient simulation would be settled to understand the startup time of the fuel cell and to study the effect of a pulse flow while using a conformal mesh. The regular and foreseeable connectivity is not seen when considering unstructured meshes. These unstructured meshes are characterized by the use of triangles elements in 2D. With regards to 3D, tetrahedra elements are used. However, quadrilateral and hexahedra elements may also be present on the mesh as it happens in this project. One of the major reasons to use an unstructured mesh is the ease of generation of the mesh. The figure 5.13 is composed by hexahedra elements regarding the surfaces with polyhedron elements when considering the volume. Additionally, one of the goals of this project was to accomplish a conformal mesh. In other words, a mesh is defined as a conformal mesh when all the interfaces of the computational domain share the same number of nodes considering the adjacent elements of the domain. Due to this, two different types of meshes will be used in the thesis to discuss and analyse the different results. The figures presented below illustrates the conformal mesh used in this thesis. A comparison between the two different meshes will be present on the following pages of this report.





**Figure 5.13:** Volume mesh of the computational domain domain near to the turbulence inducing grid



**Figure 5.14:** Volume mesh detail of the computational domain domain near to the turbulence inducing grid



**Figure 5.15:** Surface mesh of the computational domain near to the turbulence inducing grid when considering the unstructured mesh



**Figure 5.16:** Surface mesh of the computational domain near to the turbulence inducing grid when considering the structured mesh



**Figure 5.17:** Unstructured surface mesh detailed of the computational domain when considering a part of the grid



**Figure 5.18:** Structured surface mesh detailed of the computational domain when considering a part of the grid





**Figure 5.19:** Unstructured surface mesh at the inlet of the cathode



Figure 5.20: Structured surface mesh at the inlet of the cathode



# 5.6 Grid Independence Study

The grid independence study is an important part of every project related to computational fluid dynamics simulations. This study is relevant since it is important to know if the results presented are independent of the computational domain mesh. However, due to the limitation of the number of cells, there was only a partial study regarding the grid independence with four different cases. In all the



# Temperature vs Cell Count

Figure 5.21: Four different cases in order to achieve a computational domain mesh independent

simulations presented in this report, the overall mass and heat balance over all the boundaries was negligible. Moreover, a report of physical properties was analyzed to ensure the convergence of the simulations. Additionally, the residuals were low. An example is given at the of this report on the section D.



# 5.7 Boundary Conditions

As every computational fluid dynamic simulation, one of the most important parts is to set up correctly the boundary conditions with regards to the simulation. These boundary conditions are always required to solve the mathematical model. With the Matlab code presented on the Section A, the inlet conditions were defined with a specific velocity and temperature. The gas diffusion layer was set with a constant heat flux of  $2587W/m^2$  as it was presented on the section 2.8. The outlet condition was set with a pressure of zero Pascal. All the remain surfaces were set as a symmetry plane where no inputs are required. The table 5.3 gives the overview of the boundary conditions used:

Location	<b>Boundary</b> Condition	Value
Inlet	Velocity	1.004m/s
	Temperature	20 °C
Gas Diffusion Layer	Heat Flux	2587W/m <sup>2</sup>
Rest of the domain	Symmetry	No flux

#### Table 5.3: Overview of the boundary conditions

The values present above are used for the first couple of simulations. When considering subzero temperatures at the inlet, the stoichiometric ratio has to be adjusted and this adjustment will change the fluid velocity required to achieve similar performance.



# 5.8 Physics Models and Solution Methods

Table 5.4: Overview of the models and solver used in the paper

Physics Models and Solution Methods		
Turbulence Models		
Realizable k - $\epsilon$ enhanced wall treatment		
k - $\omega$ SST		
Reynolds Stresses Model		
Solution Methods		
Scheme	SIMPLE - algorithm	
Gradient	Least Squares Cell Based	
Pressure	Second Order	
Momentum	Second Order Upwind	
Energy	Second Order Upwind	
Turbulent Kinetic Energy	Second Order Upwind	
Turbulent Dissipation Rate	Second Order Upwind	
Specific Dissipation Rate(k - $\omega$ SST)	Second Order Upwind	
Reynolds Stresses	Second Order Upwind	

The SIMPLE scheme or Semi-Implicit Method for Pressure Linked Equations is an algorithm that solves iteratively the coupled pressure-velocity. The first step is to solve the momentum equation for the velocity field. However, the velocity field will not satisfy the continuity equation. The following step is to solve the Poisson equation for the pressure field. The pressure field will be used to fix the velocity field value in order to satisfy the continuity equation. Finally, and since it is an iterative process, the velocity field will not satisfy the momentum equations and the cycle has to be repetead.



### 5.9 Time Step and Courant-Friedrichs-Lewy Number

The time step is one of the most important parameters when a transient simulation is considered. This is crucial such as the time step must be smaller than a certain value in order to capture the right properties values of each cell. In order to achieve proper results, CFL number or Courant-Friedrichs-Lewy number is used to ensure a good time step is defined. The CFL number can be seen as the ratio between the fluid distance and the cell distance, mathematically illustrated by the following equation:

$$CFL = \frac{U \cdot \delta t}{\delta x} \tag{5.12}$$

Where,  $\delta t$  is the time step,  $\delta x$  is the length of a cell and U defines the free stream velocity.

# 6 Results and Discussion

In this section the results obtained from the computational fluid dynamics simulations in the project will be presented and discussed. The chapter will be divided into two sections, namely steady state simulations and transient simulations. Within the steady state simulation section, the result from the poly hexcore conformal mesh will be presented and discussed. After this, the findings from the structured non-conformal mesh will likewise be shown. Additionally, the heated turbulence inducing grid results will be introduced. Lastly, the transient simulation results acquired will be covered.

# 6.1 Steady State Simulations

Steady state simulations were done to study the different profiles such as temperature, velocity and turbulent intensity when varying the distance of the grid having the cathode inlet as a reference. Additionally, comparison studies were done for the mesh types and turbulence models.



**Figure 6.1:** Maximum temperatures of the bipolar plate, gas diffusion layer, and the fluid considering two different distances with regards to the inlet and the absence of the grid

This introductory study given in figure 6.1 was to look at the differences and the consequent effects of these distinct setups. Moreover, to look at the results obtained to calculate the maximum temperature each component and fluid would have considering the entire computational domain using the comprehensive turbulence Reynolds Stress model. It can be seen in figure 6.1, the setup where the grid was at 2.5mm from the cathode inlet was the best to set the grid in order



to achieve the lowest temperatures when considering the same given boundary conditions for the domain. This finding is also in accordance with previous experimental work on the subject(Shakhshir, Gao, and Berning 2020) Considering 2.5mm as the distance between the grid and the inlet of the cathode showed a maximum temperature of the bipolar plate of 84.85 °C. With regards to the gas diffusion layer, and considering the same setup, the maximum temperature was 90.13°C. Although promising results were acquired, the fluid temperature profile was similar for all the setups and its value was around 63.23°C. All these maximum temperature temperature temperature temperature between the setups and its value was around 63.23°C.

peratures are expected to be at the outlet as it can be seen in the figure 6.2



**Figure 6.2:** Temperature profile along the fuel cell with the boundary conditions of table 5.3 using the Reynolds Stress model

Re-scaling figure 6.2, a comprehensive analysis of the temperature gradient inside the cathode channel reveals important differences when consider those three setups. These differences are depicted in the figure 6.3. Looking at the bipolar plate temperature, it is possible to see how the placement of the grid is important to reduce the temperature along the entire domain.



**Figure 6.3:** Temperature profile (scaled) along the fuel cell with the boundary conditions of table 5.3 using the Reynolds Stress model

Having figure 6.3 as reference, it is possible to express a good cooling property when considering the domain where the turbulence inducing grid is at 2.5mm from the inlet of the cathode. The difference of temperature between the bipolar plates and the gas diffusion layers when considering "*No Grid*" domain and "2.5mm distance" is around 2.79 °C and 2.81°C, respectively.

With respect to the velocity on figure 6.4, some differences on the profiles were already expected before the simulations were done due to the different distances and the increase of the velocity of the fluid after going through the grid because of the reduction of area.

With reference to the turbulent intensity, although the maximum value is closely the same, the behaviour of the fluid presents some differences while inside the cathode channel as it can be seen when comparing the three profiles in figure 6.5 where the distance of the grid only varies 2.5mm, respectively. Due to this increase of turbulence inside the cathode channel when considering the smallest distance, 2.5mm, the heat transfer coefficient also increase leading to lower temperatures of the fuel cell components.





**Figure 6.4:** Velocity profile along the fuel cell with the boundary conditions of table 5.3 using the Reynolds Stress model



**Figure 6.5:** Turbulent intensity profile along the fuel cell with the boundary conditions of table 5.3 using the Reynolds Stress model

Figures 6.6, 6.7, and 6.8 show the temperature profiles of the bipolar plate, gas diffusion layer, and fluid respectively along the cathode channel. Comparing the three distances, it is evident that the 2.5mm distance from the cathode inlet yields the lowest temperatures. Figure 6.6 shows a bigger difference in temperature at the start of the cathode channel compared to at the end. This is reasonable, since the turbulence inducing grid will generate turbulence at the start of the channel, and thus aid in the temperature reduction of the solid materials. Further along the channel, the difference in temperature will decrease as the flow is carried further away from the grid and the turbulence induced by the grid dissipates. Figure 6.7 for gas diffusion layer profile shows the same trend as given for the bipolar plate profile with a high difference in the start due to induced turbulence, and lower difference along the channel. In figure 6.8 it can be seen that the fluid temperature has an increase in temperature. Since the flow is turbulent the mixing increases and with it the convective heat transfer.



# **Temperature Profile of Bipolar Plate**

Figure 6.6: Bipolar plate temperature profile along the cathode channel





Temperature Profile of GDL





## **Temperature Profile of The Fluid**

Figure 6.8: Fluid temperature profile along the cathode channel





**Figure 6.9:** Temperature profile along the fuel cell with the boundary conditions of table 5.3 using the Reynolds Stress model and the two different mesh types



**Figure 6.10:** Velocity profile along the fuel cell with the boundary conditions of table 5.3 using the Reynolds Stress model



**Figure 6.11:** Turbulent intensity profile along the fuel cell with the boundary conditions of table 5.3 using Reynolds Stress model and the two different mesh types



Figures 6.9, 6.10, and 6.11 show the temperature, velocity, and turbulence intensity for the RSM model respectively for both mesh types. In figures 6.9 and 6.10 where the temperatures and velocities are represented, the same trends can be observed and there seems to be small to no changes when comparing mesh types. Regarding figure 6.11 an increase in turbulence intensity can be seen in the boundary layer and this is nonphysical in nature. In addition to this, one can observe differences when comparing mesh types. However, both still predict high turbulence occurrences near the wall. This increased turbulence intensity in the boundary layer can be due to a number of reasons. Firstly, the RSM is a high Reynolds number turbulence model and is mostly applicable in highly turbulence core flows. Additionally, the RSM needs modification to capture near wall flows and is coupled with a wall function. It is most accurate when having a first cell height with  $y^+$  $\approx$  30 (Salim and Cheah 2009). Obtaining a  $y^+ \approx$  30, was not possible due to the computational domain. Secondly, when considering a heat transfer problem, it is of extreme importance to have the mesh resolved to the viscous sublayer to capture all the effects in the boundary layer. Having a  $y^+ \approx 30$  defeats this purpose. Due to these nonphysical results obtained by using the RSM, a decision was made to compare different turbulence models to investigate which would ensure best physical results.



**Figure 6.12:** Temperature profile along the fuel cell with the boundary conditions of table 5.3 while using Realizable  $k - \epsilon$  with enhanced wall treatment and the two different mesh types

Figures 6.12, 6.13, and 6.14 represent the temperature, velocity, and turbulent intensity profiles for the realizable k -  $\epsilon$  with enhanced wall treatment. Again, temperature and velocity profiles when comparing mesh types are very similar. However, when observing the turbulent intensity profiles for both mesh types in figure 6.14, one can see a difference. The difference can especially been seen close to the turbulence inducing grid and cathode inlet. The structured mesh predicts a higher turbulence intensity compare the unstructured mesh. Along the cathode channel





**Figure 6.13:** Velocity profile along the fuel cell with the boundary conditions of table 5.3 while using Realizable  $k - \epsilon$  with enhanced wall treatment and the two different mesh types



**Figure 6.14:** Turbulence intensity profile along the fuel cell with the boundary conditions of table 5.3 while using Realizable  $k - \epsilon$  with enhanced wall treatment and the two different mesh types

both have the same trend e.g. an increase in turbulence intensity as the flows moves towards the outlet. This is reasonable due to the higher temperatures further into the fuel cell. Also worth noticing is that a boundary layer can be observed close to the wall. These are realistic, since the flow will always be laminar in the close vicinity of the wall, namely in the viscous sublayer. However, when investigating the turbulence intensity, extremely high percentages can be seen.





**Figure 6.15:** Temperature profile along the fuel cell with the boundary conditions of table 5.3 using the k- $\omega$  SST model and the two different mesh types



**Figure 6.16:** Velocity profile along the fuel cell with the boundary conditions of table 5.3 using the k- $\omega$  SST model and the two different mesh types



**Figure 6.17:** Turbulence intensity profile along the fuel cell with the boundary conditions of table 5.3 using the k- $\omega$  SST model and the two different mesh types



Figures 6.15, 6.16, and 6.17 show the temperature, velocity, and turbulence intensity profiles for the SST k -  $\omega$  turbulence model. Again, the temperature and velocity profiles are very similar and are in the same order of magnitude. Comparing both mesh types when considering turbulence intensity is seen to be quite different. The turbulence intensity in the unstructured mesh is smaller in magnitude, but does have similar trend along the cathode channel. Additionally, small turbulence seems to be created by the grid compared to the other mesh type. The structured mesh type shows higher turbulence created by the grid entering the cathode. In addition to this, a clear boundary layer can be seen, where the highest turbulence is in the core flow and laminar flow is closest to the wall.

#### **Results Summary**

Concerning the mesh types used, the structured hexahedral mesh seems to be a better fit for the current computational domain. Since the computational domain is fairly simple and velocity flow directions are well defined, there should not be need of a complex unstructured mesh, since this would only induce a larger numerical error. The poly hexcore mesh shows some inconsistencies compared to the hexahedral mesh regarding the boundary layer. With the regards to the turbulence models, results show RSM to be inconsistent, since an increase in turbulence intensity is generated in the boundary layer regarding both mesh types and these results are nonphysical. Realizable k -  $\epsilon$  coupled with enhanced wall treatment gives reasonable predictions, where a laminar viscous flow can be seen closest to the wall and turbulence in the core flow. However, the magnitude of turbulence intensity seems to be rather high, peaking at 65 % . Lastly, the SST k -  $\omega$  was investigated and results show realistic profiles in terms of temperature, velocity, and turbulence intensity. Similar to realizable k -  $\epsilon$  with enhanced wall treatment, the SST k -  $\omega$ captures correctly the flows in the boundary layer close to the wall. For the SST k -  $\omega$  the turbulence intensity does not reach unrealistically high values having the maximum around 10 %. Moreover, the SST k -  $\omega$  is designed to be predict correct behaviour near the wall. Based on the results obtained the structured hexahedral mesh with SST k -  $\omega$  turbulence model seems to give the most accurate results.

## 6.1.1 Heated Turbulence Grid in Subzero Conditions

The results concerning the heated grid calculations and simulations will be considered in this section. The section is separated into 4 parts, where the 4 grid dimensions will be considered in their respective subsections. The MATLAB script used in the calculations is given in appendix A. For the following simulations a 0.9557m/s velocity was consider at the inlet.

## Grid A

Grid A is the first grid dimension considered. This grid acts as the benchmark, since it was used by the previous groups, which conducted similar studies to this. This was described in section 4.1 As previously described in section 3 the solid volume is given as  $4.935 \text{ }mm^3$ .

Table 6.1 gives a handy overview of the heated grid simulations done. In total five different steady state simulations were done. The changing parameter was the temperature difference across the grid and thus the heat input to the grid.

Inlet Air Velocity [m/s]	Heat Input[W]	$\Delta T$ Across Grid [°C]	Grid Temperature [°C]
0.9557	0.3268	25°C(-20°C to 5°C)	1511°C
0.9557	0.2615	20°C(-15°C to 5°C)	1223°C
0.9557	0.1961	15°C(-10°C to 5°C)	928°C
0.9557	0.1307	10°C(-5°C to 5°C)	626°C
0.9557	0.0654	5°C(0°C to 5°C)	319°C

Table 6.1: Resulting grid surface temperatures for grid dimension A in the CFD simulations

Since the solid volume of grid A is relatively small, it is clear from figure 6.18 that the resulting grid surface temperature is very high and peaks at a temperature of 928 °C. This resulting temperature is considered high, since the surrounding temperatures of air, gas diffusion layer, and bipolar plate are low in comparison. In figure 6.19 the preheating of the incoming air can be seen. The incoming air has a inlet temperature of -10°C. The cold air reaches the grid and as it flows through it gets heated up via convection and reaches an approximate value of 5°C after the grid as depicted.




**Figure 6.18:** shows the temperature of grid A, when the temperature difference across the grid is 15°C. The turbulence inducing grid is a distance of 2.5mm from the cathode inlet.



**Figure 6.19:** shows the air temperature as the air passes through grid A. The turbulence inducing grid is a distance of 2.5mm from the cathode inlet.

### Grid B

Similarly to grid A in the previous subsection, grid B and the results obtained from the simulations will be covered here.

Grid B has a grid depth of 2mm compared to 1mm in grid A. This means a higher solid volume and thus also a decrease in grid surface temperature, since the heat input is implemented to a larger volume. This can be seen on figure 6.20. The grid

Inlet Air Velocity [m/s]	Heat Input[W]	$\Delta T$ Across Grid [°C]	Grid Temperature [°C]
0.9557	0.3268	25°C(-20°C to 5°C)	863°C
0.9557	0.2615	20°C(-15°C to 5°C)	699°C
0.9557	0.1961	15°C(-10°C to 5°C)	531°C
0.9557	0.1307	10°C(-5°C to 5°C)	359°C
0.9557	0.0654	5°C(0°C to 5°C)	184°C

Table 6.2: Resulting grid surface temperatures for grid dimension B in the CFD simulations



**Figure 6.20:** shows the temperature of grid B, when the temperature difference across the grid is 15°C. The turbulence inducing grid is a distance of 2.5mm from the cathode inlet.

surface temperature is approximately 531°C.

Referring to table 6.2, it is clear that the grid surface temperatures are lower than for Grid A. This is a result of increased solid volume of the grid. Although, the temperatures represented in 6.2 are lower than in table 6.1, they are still considered too high. This is due to the fact that the grid will be situated right next to the fuel cell channel and the sole purpose of the air cooling is to the decrease the temperature of the fuel cell channel. The aim is to have a max grid surface temperature of around 200-300°C.





**Figure 6.21:** shows the air temperature as the air passes through grid B. The turbulence inducing grid is a distance of 2.5mm from the cathode inlet.

#### Grid C

Inlet Air Velocity [m/s]	Heat Input[W]	$\Delta T$ Across Grid [°C]	Grid Temperature [°C]
0.9557	0.3268	25°C(-20°C to 5°C)	982°C
0.9557	0.2615	20°C(-15°C to 5°C)	799°C
0.9557	0.1961	15°C(-10°C to 5°C)	608°C
0.9557	0.1307	10°C(-5°C to 5°C)	412°C
0.9557	0.0654	5°C(0°C to 5°C)	211°C

Table 6.3: Resulting grid surface temperatures for grid dimension C in the CFD simulations

Figures 6.22 and 6.23 show the grid temperature and air temperature around the heated grid. Comparing theses figures to the previous figures regarding the same topic, a temperature decrease can be seen when considering 6.1 and 6.3. This again is due to the increased solid volume of grid A compared to grid C.





**Figure 6.22:** shows the temperature of grid C, when the temperature difference across the grid is 15°C. The turbulence inducing grid is a distance of 2.5mm from the cathode inlet.



**Figure 6.23:** shows the air temperature as the air passes through grid C. The turbulence inducing grid is a distance of 2.5mm from the cathode inlet.

### Grid D

Grid D is the final grid dimension considered and is simultaneously the grid with the largest solid volume.

Table 6.4: Resulting grid surface temperatures for grid dimension D in the CFD simulations

Inlet Air Velocity [m/s]	Heat Input[W]	$\Delta T$ Across Grid [°C]	Grid Temperature [°C]
0.9557	0.3268	25°C(-20°C to 5°C)	562°C
0.9557	0.2615	20°C(-15°C to 5°C)	472°C
0.9557	0.1961	15°C(-10°C to 5°C)	348°C
0.9557	0.1307	10°C(-5°C to 5°C)	236°C
0.9557	0.0654	5°C(0°C to 5°C)	122°C



**Figure 6.24:** shows the temperature of grid D, when the temperature difference across the grid is 15°C. The turbulence inducing grid is a distance of 2.5mm from the cathode inlet.

As for the previous grid dimensions, the grid temperature and air temperature around the grid are also represented for grid D. Shifting the focus to figure 6.24, it can be seen that the grid surface temperatures is approximately 348°C. This a temperature decrease of 580°C, when comparing to the grid surface temperature of grid A considering the same temperature difference across the grid.



**Figure 6.25:** shows the air temperature as the air passes through grid D. The turbulence inducing grid is a distance of 2.5mm from the cathode inlet.

### Heated Turbulence Inducing Grid - Power Usage

Fuel Cell Power[W]	Grid Heat Input[W]	∆T Across Heated Grid [°C]	Percentage [%]
0.4378	0.3268	25°C(-20°C to 5°C)	74.66
0.4378	0.2615	20°C(-15°C to 5°C)	59.73
0.4378	0.1961	15°C(-10°C to 5°C)	44.80
0.4378	0.1307	10°C(-5°C to 5°C)	29.86
0.4378	0.0654	5°C(0°C to 5°C)	14.93

### Table 6.5: Grid Power Used Compared Fuel Cell Power

#### 6.1.2 Results summary

The previous subsections, regarding placing a heated turbulence inducing grid in front of the cathode channel, show reasonably good and practical results concerning its feasibility. Grid A shows fairly high grid surface temperatures ranging from 319°C to 1511°C depending on the temperature difference across the grid. For a temperature decrease of 5°C, the grid surface temperature has a resulting value



of 319°C, which is high, since the goal is to have a surface temperature of 200°C - 300°C. Grid B, which gives a temperature range of 184°C - 863°C has a temperature decrease when comparing grid A, but still does have high surface temperatures, when the temperature difference across the grid increases to more than 5°C. Considering grid C and grid D, there can be seen an additional temperature decrease since, these increase the solid volume part of the grid. Grid C ranging from 211°C - 982°C and grid D ranging 122°C - 562°C show decent surface temperature, but are also at the high end of the aim. Grid C has a temperature of 412°C considering a 10°C preheating of incoming air, while grid D shows a temperature of 236°C. In addition, grid D also has a temperature of 348°C at a 15°C temperature difference across the grid.

It can therefore be concluded that placing a heated turbulence inducing grid before the cathode, to preheat the air is feasible and reasonable to some extent. With the current grid dimensions, preheating the incoming air by more than 10°C is not feasible, since the grid surface temperature will be too high and can potentially harm the fuel cell channel or to some extent deteriorate parts of the fuel cell. In addition to this, another crucial factor is the power used for heating the grid compared to the fuel cell channel. It is favourable to use around 10% - 20% of the total power produced by the fuel cell. Considering table 6.5 it is clear that preheating the incoming air by 10°C gives approximately 30% grid power usage compared to the total power. It can be therefore be concluded, both from a temperature but also power perspective, that a turbulence inducing heating grid preheating the incoming air by 10°C and lower is a feasible solution under current grid dimensions and circumstances.



### 6.2 Transient Simulations

In this section, the transient simulation will be analyzed and discussed. The main goals of the transient simulation carried out during this project was to study the effect of having a pulse flow and, additionally, to know the start-up time of the system, the amount of time required to reach stead state conditions. The pulse flow was modeled having a period of ten seconds and a maximum variation of intensity of 20%. The following equation illustrates the profile

$$u_{inlet} = 1.004 + 1.004 \cdot 0.2 \cdot sin(0.6283t); \tag{6.1}$$

where t represents the time of the of the flow. As it can be seen from the figure 6.26, the start-up time of the fuel cell is around 470 seconds. After the first 470 seconds the temperature starts to stabilize around the same numbers. Even though



**Figure 6.26:** Maximum temperatures during a transient simulation considering a distance of 2.5mm between the grid and the cathode inlet and with a pulse flow defined on the equation 6.1

the results can be found interesting due to the different temperatures acquired it seems the pulse flow does not have a strong effect on the temperature profile since the average value will be undeniably close to the value obtained when considering a constant inlet velocity of 1.004m/s.

The figure 6.27 illustrates the change in temperature of the fuel cell when it starts to operate until it reaches a statistically steady state. It is possible to see how the gradient of the temperature changes from the inlet to the outlet along the time.



Figure 6.27: Temperature profile along the X-Y plane (z=0.002025m) during the first six minutes.

One of the goals of the project was to analyse if a pulse flow would give a better cooling of the fuel cell. The period of the sinusoidal function was ten seconds and the amplitude would change 20% from the average free stream value. The following figure, figure 6.28, illustrates the last 70 seconds of the transient simulation. It is possible to see, statistically steady state conditions were reached. However, the fluctuations of the temperature represented by the blue line are just a result of the



velocity variation at the inlet. When the velocity was 20% higher than the average, the temperature would decrease - a trough. As soon the velocity would decrease to its minimum value of  $\approx 0.80$  m/s the maximum temperature would be reached - a peak. Finally, it can be seen the average mean temperature from the transient simulation is close to the steady state simulation temperature.



### Gas Diffusion Layer Temperature

**Figure 6.28:** Last 70 seconds of the transient simulation where statistically steady state conditions were reached but there was no significant cooling effect when compared to the steady state temperature.



### 7 Conclusion

The numerical methodology used in the thesis was successful in validating previous experimental work on the subject. For the turbulence inducing grid, a distance of 2.5 mm from the cathode inlet was shown to be most effective, where most turbulence was created and thus the highest cooling effect. At best, a temperature reduction in the gas diffusion layer of  $\approx 2.8$  °C could be obtained. The comparison study between the unstructured poly hexcore mesh and structured hexahedral mesh showed the latter mesh type to be the most effective and precise. This conclusion could be blamed on different reasons. Firstly, the computational domain used was rather simple and clear velocity directions were given. Creating a complex mesh for a simple geometry will in general induce higher numerical error. Secondly, since the problem at hand was convective heat transfer, resolving the mesh down to the viscous sublayer was of great importance to capture accurate results within the boundary layer. This was easier obtained with the structured hexahedral mesh. The comparison study for the turbulence models showed some inconsistencies with the RSM model. High turbulence intensity was created in the boundary layer which is nonphysical. In general, the RSM model is a high Reynolds number turbulence model and is primarily used in high turbulence core flows. Most accurate results are obtained by combining the RSM model with a wall function, where the first cell height is given a  $y^+$  value of  $\approx 30$ . These  $y^+$  values could not be achieved in the study, since it was limited by the computational domain. Furthermore, having a  $y^+$  of  $\approx 30$  would defeat the purpose of investigating heat transfer inside the cathode channel. Best results were achieved by using the SST k -  $\omega$  turbulence model. Regarding the heated turbulence inducing grid, feasibility was concluded to some extent. The best results obtained were for grid D and with preheating the air by 10°C. The resulting grid surface temperature obtained using this setup was  $\approx$  236°C. In addition to this the grid would require  $\approx$ 30 % of the total fuel cell power. For the unsteady flow conditions, the conformal unstructured poly hexcore mesh together with RSM was used and no remarkable temperature reduction in the fuel cell solid materials was seen, when varying the inlet velocity by 20%. This result was rather surprising, but could again be due to the possibly induced numerical errors from the mesh and the inconsistency of the RSM model regarding the nonphysical increased turbulence intensity within the boundary layer. Furthermore, the fuel cell startup time was  $\approx$  470 seconds until the desired steady state temperature was reached.

### 8 Future Work

Based on the findings in this thesis, several topics could be even more developed and studied in order to achieve better proton exchange membrane fuel cell performances and more realistic results.

- The gas diffusion layer could have a higher level of modelling due to its porosity and physical properties.
- A different periodic boundary condition could be applied changing the period of the function and its amplitude in order to study the cooling effect when applying a pulse flow.
- An experimental setup could be developed in order to measure directly the temperatures of the fluid along the channel to have a better comparison between the turbulence models and their values.
- A more refined structured mesh could be used for all the simulations including the transient one.
- A different design for the fuel cell could be modelled in order to increase the performance of the cell.



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### A Matlab Script

```
%
1
  clear all
2
  clc
3
4
  %Constants
5
  RH= 0 ; % Relative Humidity
6
  F = 96487 ; % Faradays constant [C/mol]
7
  R=8.314472; % universal gas constant [J/(K*mol)]
8
  % Areas
10
  A_ch = 3.4088*10^{(-6)}; % fluid channel area [m<sup>2</sup>]
11
  A_gdl = 189*10^{(-6)};
                         % gas diffusion layer area [m<sup>2</sup>]
12
  A_duct = 10.935*10^{(-6)}; % inlet duct area [m<sup>2</sup>]
13
14
 %Molar Mass
15
 M_oxygen = 32; % molar mass of oxygen
16
 M_nitrogen = 28; % molar mass of nitrogen
17
  M_hydrogen = 2; % molar mass of hydrogen
18
  M_water = 18; % molar mass of water
19
20
  %Current Density
21
  i_density = 3850; % [A/m^2]
22
23
  %Stoichometric Flow Ratio
24
  epsilon_cat= 51; % Stoichiometric flow ratio for air at
25
      cathode
  epsilon_ano= 1.1; % Stoichiometric flow ratio for hydrogen at
26
       anode
27
  % Pressure and temperatures
28
  p_amb= 101325 ; % ambient pressure [Pa]
29
  T_inlet = 5;
                  % temperature inlet [C]
30
  T_inletK = T_inlet + 273.15; % temperature inlet [K]
31
  T_outlet = [30:10:100] + 273.15; % temperature outlet vector
32
      [K]
33
  %Oxygen Mole fraction
34
  x_oxygen = 0.21;
35
36
```



```
% Antoine's equation
37
 A = 8.07131;
38
 B = 1730.63;
39
 C = 233.426;
  D = 133.233;
41
  p_{sat} = D * 10^{(A-(B/(C+T_inlet)))}; %saturation pressure [Pa]
42
43
  % Enthalpies using CoolProp and Tables at inlet temperature
44
  h_oxygen_in = py.CoolProp.CoolProp.PropsSI('H', 'P', p_amb, 'T',
45
      T_inletK , 'O2') / 1000 * M_oxygen;
  h_hydrogen_in = py.CoolProp.CoolProp.PropsSI('H', 'P', p_amb, 'T
46
       ,T_inletK , 'H2') / 1000 * M_hydrogen;
  h_nitrogen_in = py.CoolProp.CoolProp.PropsSI('H', 'P', p_amb, 'T
47
      ',T_inletK , 'N2')/ 1000 * M_nitrogen;
  h_water_vapour = [10072.512, 10408.829, 10745.829]
48
      11083.146 , 11421.146 , ...
  11759.780 , 12099.463 , 12439.097 , 12780.414 , 13122.414 ,
49
      13464.731];
50
  for i = 1:8
51
   % Enthalpies using CoolProp and Tables at outlet
52
       temperatures
  h_oxygen(i) = py.CoolProp.CoolProp.PropsSI('H', 'P', p_amb, 'T',
53
      T_outlet(i), 'O2')/ 1000 * M_oxygen;
  h_hydrogen(i) = py.CoolProp.CoolProp.PropsSI('H', 'P', p_amb, 'T
54
       ,T_outlet(i), 'H2')/ 1000 * M_hydrogen;
  h_nitrogen(i) = py.CoolProp.CoolProp.PropsSI('H', 'P', p_amb, 'T
55
      ',T_outlet(i),'N2')/ 1000 * M_nitrogen;
56
57
  % Calculations of fuel cell voltage following 1st law of
58
     thermodynamics
   Vcell(i) = (((1/(4*F)) * (epsilon_cat) * (h_oxygen_in - 8682))
59
        + . . .
       ((1/(4*F)) * (3.762*epsilon_cat) * (h_nitrogen_in - 8669)
60
          ) + . . .
       ((1/(2*F)) * (epsilon_ano) * (h_hydrogen_in - 8468)) +...
61
       + ((((RH) / ((p_amb/p_sat)-RH)) * (1/0.21) * ((epsilon_cat)
62
          /(4*F)))))...
        -(((1/(4*F)) * (epsilon_cat - 1) * (h_oxygen(i) - 8682))
63
           + . . .
```

```
((1/(4*F)) * (3.762*epsilon_cat) * (h_nitrogen(i) - 8669)
64
          ) + . . .
       ((1/(2*F)) * (epsilon_ano -1) * (h_hydrogen(i) - 8468))
65
          + . . .
       (((RH) / ((p_amb/p_sat) - RH)) * (1/0.21) * ((epsilon_cat))
66
          /(4*F)) + (1/(2*F))) *...
       (-241820 + h_water_vapour(i) - 9904));
67
68
  end
69
70
  %Velocity at cathode inlet, B [m/s]
71
  u_b = epsilon_cat*(i_density/(4*F))*A_gdl*((R*T_inletK)/(
72
     x_oxygen*p_amb*A_ch));
73
  %Velocity at the inlet of the duct, A [m/s]
74
  u_A = u_b * A_ch/A_duct;
75
76
 %% HEATED GRID
77
  T_before_cathode=5; %temperature before the cathode inlet [C]
78
  density = 1.2466; % density [kg/m^3]
79
  spec_heat = 1.0035; % specific heat capacity of air at
80
      constant pressure [J/(g*K)]
  delta_T = T_before_cathode - (-20); \% temperature difference
81
      across grid [C]
  Vol_grid = 4.935*10^{(-9)}*2; \% volume of grid [m<sup>3</sup>]
82
  flow_rate = density*u_A*A_duct*1000; % calculated flowrate [
83
     kg/s]
84 Q = flow_rate*spec_heat*delta_T; % heat input to grid [W]
  Heat_Gen = Q/Vol_grid; % heat generation uniformally
85
      distributed in turbulence grid [W/m^3]
  Power_fcell = Vcell(2)*i_density*A_gdl ; % power of fuel cell
86
       [W]
  percentage = Q/Power_fcell *100; % power usage of grid
87
     compared to fuel cell in percentage [%]
```



### **B** Prisms Layer Calculations

As it was explained in this report, the mesh quality it is one of the most important part when considering the pre-processing of a computational fluid dynamics simulation. While studying the fluid behaviour, an important phenomena that is required to take into account is the boundary layer. There two main types of boundary layers: the velocity boundary layer and the thermal boundary layer. With regards to the velocity boundary layer, the no-slip condition at the wall, near the wall the fluid velocity will be zero. The absence of motion of this layer will decrease the velocity of the adjacent particles due to the friction existent between them. This wall will affect the velocity profile of the fluid until a certain distance. This region is called the velocity boundary layer. With respect to the thermal boundary layer the behaviour is quite similar to the previous one. This boundary layer will be originate when the fluid at a certain temperature flows over an object with a different temperature. To have an idea of this phenomena while analyzing a final result, the mesh is required to be fine near the wall. To acquire such requirement there is the need to add prism layers. This prism layers are placed near the wall after their first height cell is calculated. To determine the value of the first height cell, Reynolds number, wall shear stress,  $\tau_{wall}$ , and a desired y<sup>+</sup> are some of the properties needed White 2016.

$$Re_x = \frac{\rho \cdot U \cdot L}{\mu} \tag{B.1}$$

Reynolds number is obtained by the previous equation. After the Reynolds number is calculated, there are several options to get the friction coefficient such as Colebrook equation or Moody's Diagram or an explicit correlation:

$$C_f = \frac{0.026}{Re_x^{\frac{1}{7}}}$$
(B.2)

The next step is to calculate the wall shear stress which can be done using the following equation

$$\tau_{wall} = \frac{C_f \cdot \rho \cdot U^2}{2} \tag{B.3}$$

Lastly, the factor required to obtain the first cell height, friction velocity, is given by the equation:

$$U_{fric} = \sqrt{\frac{\tau_{wall}}{\rho}} \tag{B.4}$$

The following expression gives the value of the first cell height corresponding to the  $y^+$  desired:

$$\Delta s = \frac{y^+ \cdot \mu}{U_{fric} \cdot \rho} \tag{B.5}$$



## C Mesh Quality Statistics For The Simulations

The table C.1 illustrates the values of the orthogonal quality, aspect ratio and skewness of this project. All this properties were described previously on the section 5.5.

**Table C.1:** Overview of the mesh quality statistics for all the different computational domains considered in this thesis

Mesh Quality Statistics	Ortho	gonal Q	uality		Aspect Ra	tio		Skewnes	8 <b>S</b>
Computational Domain	Min	Avg	Max	Min	Avg	Max	Min	Avg	Max
2.5mm	0.200	0.9673	1.000	1.000	11.42	1.778	0	0.0327	0.7999
5mm	0.200	0.973	1.000	1.000	1.622	10.551	0	0.0268	0.7995
No Grid	0.203	0.961	1.000	1.000	6.288	1.882	0	0.797	0.039
Structured 2.5mm	0.443	0.999	1.000	1.000	14.88705	97.31783	0	0.0029235	0.7951747



## **D** Convergence Criteria

In this project, the convergence criteria was respected for all the simulations where the residuals were consistently low and a second physical parameter such as the maximum temperature of all the components of the fuel cell. The following figures are from a simulation using the Realizable  $k - \epsilon$  with enhanced wall treatment and the 2.5mm computational domain:



**Figure D.1:** Residuals used as a convergence criteria on a simulation using the Realizable  $k - \epsilon$  with enhanced wall treatment



**Figure D.2:** Temperature parameter used as a convergence criteria on a simulation using the Realizable  $k - \epsilon$  with enhanced wall treatment

# **E** Fluent Settings

	Turbulence inducing grid before the cathode inlet
General Setup	
Pressure Based	\[         \]     \[         \[         \]     \[         \]     \[         \[         \]     \[         \]     \[         \[         \]     \[         \[         \]     \[         \[         \]     \[         \[         \[         \[
Steady-State	$\checkmark$
Gravity [m/s <sup>2</sup> ]	-9.81
Models	
Reynolds Stress Model	4
k-ω SST	$\checkmark$
Realizable k- $\epsilon$ enhanced wall treatment	$\checkmark$
Zones	
Air	Fluid
Bipolar Plate	Solid
Gas Diffusion Layer	Solid
Grid	Solid
Outside Air (before grid)	Fluid
Outside Air (after grid)	Fluid
Boundary Conditions	
Inlet (velocity inlet) [m/s]	1.004
Inlet (Temperature) [°C]	20 °C
Outlet (pressure outlet) [Pa]	0
HeatFlux	$2587W/m^2$
Solution Methods	
Scheme	SIMPLE - algorithm
Gradient	Least Squares Cell Based
Pressure	Second Order
Momentum	Second Order Upwind
Turbulent Kinetic Energy	Second Order Upwind
Turbulent Dissipation Rate	Second Order Upwind
Specific Dissipation Rate	Second Order Upwind
Reynold Stresses	Second Order Upwind

### Table E.1: Overview of the Fluent settings