

---

**Numerical study of the predictive capabilities of  
Reynolds Averaged Navier-Stokes (RANS)  
turbulence models applied to catalytic converters**

---

Student: Nour Sánchez Abad

Supervisor: Humberto Medina

Coventry University

320 EKM: Project

25/04/2016

**Abstract**

Air pollution is a constantly growing concern that industry and organisations need to face nowadays. It has been demonstrated that one of the major factors that contributes to the level of the air pollution comes from the automotive sector. As a response to the raised claim, the industry developed new types of devices to reduce the emissions.

This project deals with the analysis of one of these components that is the catalytic monolith using the method of Computational Fluid Dynamics (CFD) and a further benchmark of the results obtained against the experimental data. An ideal configuration of an ideal monolith is being used to perform the analysis with RANS computational model of approach. In addition to this model,  $v^2 - f$ , Launder-Sharma, and  $k_t - k_l - \omega$  turbulence models are applied and the solutions will be tested by means of OpenFOAM simulations.

It is examined the effect that common numerical discretisation schemes for the gradient and the divergence term as well as the input conditions have on the resulting velocity profile.

### **Acknowledgments**

I would like to acknowledge this report to my supervisor Humberto Medina and appreciate his support during the development of my project.

## INDEX

---

1	Chapter 1. Background .....	4
1.1	Introduction.....	4
1.2	Aim and Objectives.....	6
1.3	Structure of the project.....	7
2	Chapter 2. Literature Review.....	8
2.1.	Introduction.....	8
2.2.	Theoretical and experimental studies.....	8
2.3.	Computational Fluid Dynamics studies .....	10
2.4	Conclusion .....	24
3	Chapter 3. Research Approach.....	25
3.1	Introduction.....	25
3.2	Research Methods.....	25
3.2.1	Research process and philosophy .....	25
3.2.2	Research Methodology.....	26
3.2.3	Data Collection .....	27
4	Analysis of results .....	28
4.1	Introduction.....	28
4.2	Methodology .....	28
4.3	Case set-up .....	29
4.4	Results .....	31
4.4.1	$v2 - f$ turbulence model.....	31
4.4.2	$kt - kl - \omega$ turbulence model.....	34
4.4.3	Launder-Sharma turbulence model .....	36
4.5	Conclusion .....	37
5	Conclusion and recommendations.....	38
5.1	Conclusion .....	38
5.2	Further work and recommendations .....	39
	List of references .....	40
	Appendix I –Project Management.....	46
	Appendix II – Project proposal .....	1
	Appendix III - Ethics approval certificate.....	6
	Appendix IV – Log Book.....	8

# 1 CHAPTER 1. BACKGROUND

---

## 1.1 INTRODUCTION

Air pollution is one of the most serious issues that is needed to be considered nowadays. The contaminant particles which are suspended on air are harmful and even more, they detrimentally affect to the environment as well as the human health, causing an undesirable impact. That is why, numerous studies focused on the different sectors of the Industry that presents high levels of emissions to the atmosphere. As a result, it was seen that one of the major sectors which produces a high percentage of pollutants is the transport sector, mainly due to the fuel combustion that takes place within the automotive engines.

In order to provide a solution for this problem measurement were needed to be taken. The institutions elaborated a series of emission regulations so as to minimize the problem worldwide. According to Hagevik (1970), the first legislation measurement which dealt with control of automotive exhaust gas emissions was introduced in California in 1947, rapidly followed by other important locations.

Considering the circumstances, the automotive sector needed to provide a series of solutions so as to reduce the air pollution levels produced by the engines which could comply the requirements set by legislative bodies. Diverse research was made in terms of fuel combustion as well as possible components which could minimize the exhaust gases. One of the most important devices which were developed to deal with this situation was the catalytic monolith (Searles et al. 2002).

The catalytic converter is an after-treatment device which is located after the automotive engine which converts the exhaust gases. It usually is of a monolith and a diffuser which is connected to the exhaust pipe from the engine.

The monolith consists of a structure with numerous parallel channels with a small hydraulic diameter of around 1mm and square cross section areas. These channels are coated with a thin wash coat of precious metals which allow the system to achieve the activation energy and undertake a series of chemical reactions (Patel et al. 2012).

As mentioned, the main function of the catalytic converter consists of the reduction of the exhaust gases which are emitted from the combustion process of the engine. According to Yamin (2012) the most common harmful gases are known to be unburned hydrocarbons (HC), carbon monoxide (CO) and nitrous oxides (NO<sub>x</sub>). These emissions are treated in the monolith through the chemical reactions and the result consist of their conversion into carbon dioxide (CO<sub>2</sub>), water vapour (H<sub>2</sub>O) and nitrogen (N<sub>2</sub>), gases which are respectively less hazardous.

The proper design of the catalytic converter is essential in order to achieve a good efficiency in the conversion process. Either the shape or size of the monolith depends on the vehicle size or packaging constraints, so it is not stipulated (Porter et al., 2014). The monoliths are desired to be as shorter as possible due to the backpressure and the pressure drop through it, which is tried to be minimized. Nevertheless, enough surface is needed in order to ensure that the conversion process can occur, thus a diameter higher than the exhaust pipe is required.

This is the reason why a diffuser is needed in order to connect the front face of the monolith with the exhaust pipe as shown in Fig.1 :

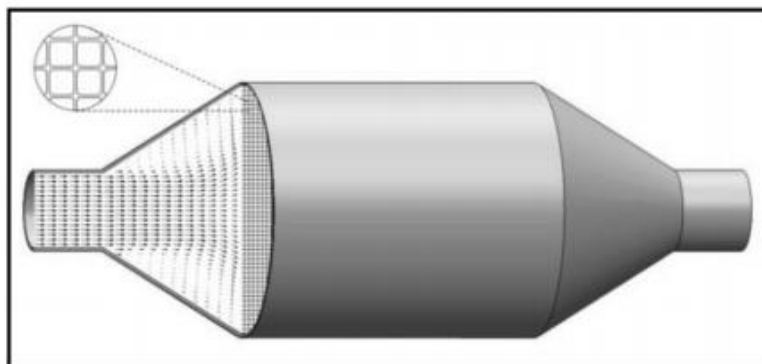


Figure 1. Catalytic monolith with a diffuser (Porter et al. 2014)

Axisymmetric wide angled diffuser however led to a secondary inconvenient that needed to be considered, which is the non-uniform flow.

Benjamin et al. (1996) estimated that malfow distribution can lead to premature deactivation of the monolith at those areas with high flow. Therefore, a decrease of the conversion efficiency of the gases and an increase of pressure loss is observed, which means a poor performance of the catalyst. Due to this reason, the analysis and prediction of flow distribution within the catalytic has become essential subjects that are desired to be developed.

Computational Fluid Dynamics (CFD) is a recent procedure that was included in engineering analysis and is widely used in the industry as well as in the investigation sector. It has been used to assess the efficiency and performance of catalytic converters.

It was mainly developed in the 80s and it represents a set of numerical tools to analyse the behaviour of component with a defined configuration under determined initial and boundary conditions with a selected computational model of approach. The main purpose of CFD is to recreate a desired scenario represented by the set-up conditions thought simulations that allows assessing the efficiency and performance of the component (Liu et al., 2003).

Furthermore, there exists different computational model of approach based on the resolution of the fundamental equations of fluid mechanics. A widely-used model that combines the advantages of accuracy and good computational cost is the Reynolds-averaged Navier-Stokes (RANS). This model provides an averaged solution which is based on mean and fluctuating factors, aspect that represents a limitation that needs to be considered. In addition to this model, turbulence approach models are applied that implement the turbulent predictions.

In terms of the flow regime, the flow within the catalytic converters is not uniform and turbulence models are needed to be applied in the simulations undertaken. The models are mainly based on different ways of modelling the turbulence viscosity.

## 1.2 AIM AND OBJECTIVES

This project aims to find an adequate CFD turbulence model of approach that could well predict the flow distribution within a simplified two-dimensional catalytic converter in conjunction with RANS model, assuming the monolith as a porous medium. The main questions that are attempted to answer are:

- How does the choice of discretisation scheme affect the CFD results provided by the  $v^2 - f$  model?
- How accurate are state-of-the-art RANS models in predicting the flow within an idealised catalytic converter (benchmarked against experimental data)?
- Will a transition-capable RANS model ( $k_t - k_l - \omega$ ) lead to improved CFD predictions?

Moreover, the objectives of this project are the following:

- To carry out a critical literature review to appraise the state-of-the-art in relation to CFD applied to emission after-treatment devices.
- To gain a solid analysis of the assumptions behind RANS modelling and 3 target turbulence models.
- To investigate the effect that common numerical discretisation schemes for the gradient terms of the turbulence models have on the numerical solution.
- To investigate the effect that selected upwind numerical discretisation schemes for the divergence terms of the turbulence models have on the numerical solution.
- To evaluate at least 3 low Reynolds RANS models applied to an idealised catalyst configuration.
- To discuss the results obtained and compare them with the experimental data. The variation of pressure and velocity will be examined.
- To highlight the key findings from this work and provide the proper recommendations.

## 1.3 STRUCTURE OF THE PROJECT

This report follows a structure divided in four different chapters with respective purposes;

- **Chapter 1. Introduction**

An overview of the project is presented. This section provides an insight in the topic and states the aim, research questions and objectives that this project intends to cover.

- **Chapter 2. Literature review**

This section illustrates a critical review of the literature. It provides an insight on previous research and the basics of this research are explained and compared. As a result, a solid explanation is delivered and essential key aspects are highlighted in order to gain a critical understanding about the research topic.

- **Chapter 3. Analysis of results**

This section consists on the analysis and discussion of the results obtained. The validation of these is also performed and commented.

- **Chapter 4. Conclusion and recommendations**

This section concludes and summarises the research performed. Additionally, the key findings related to the aim and objectives of this project are highlighted. Finally, it provides a series of recommendations based on the outcomes obtained.



## 2 CHAPTER 2. LITERATURE REVIEW

---

### 2.1. INTRODUCTION

The complexity of flow distribution within a catalytic converter, consisting of a set of physical phenomena occurring within a turbulent flow and thus areas of knowledge such as fluid dynamics, thermodynamics, heat and mass transfer and chemical kinetics must come together in an attempt to model the distribution of the flow. Computational fluid dynamics is presented as a useful tool which allows predicting these phenomena. Therefore, this chapter presents a review of the key literature on the topic from the most fundamental aspects to some of the most contemporary tendencies.

### 2.2. THEORETICAL AND EXPERIMENTAL STUDIES

Since Catalytic converters appeared there have been several investigations with the aim of improving their performance focusing in the analysis of the flow distribution. As mentioned before, this is mainly due to the fact that catalytic converters supposed a necessary advance in terms of exhaust gases control in order to minimize the toxic emissions in the environment produced by automotive engines and therefore complying the legislation (Heck 1995).

In order to better understand the flow distribution within the converter, analysis were focused on the design so as to evaluate the effect of the geometry. Examples of this can be found in the work done by researches such as Comfort (1974), Howitt and Sekella (1974), Lemme and Givens (1974), Zygourakis (1989), Weltens et al. (1993), Benjamin et al. (1996).

It was observed that the flow entered the diffuser as a jet and did not follow the wall's divergent shape, in other words, the flow suffered a separation from the walls. Additionally, as the jet approaches to the front face of the monolith it suffers a deceleration in the axial direction and also part of the flow is deviated in the radial direction. As a result, part of the flow is able to enter into the channels and the rest is spread through the empty spaces as shown in Fig.2 and Fig.3, creating two recirculation bubbles upwards and downwards of the main jet motion. The highest velocity is found at the centre-line of the jet which enters the channels axially, however at higher angles of it approaches the cannels obliquely and the resistance increases.

Therefore, the design resulted a decisive factor in the performance and the effectiveness of its applications. Poor flow distribution led to higher system losses, deterioration, reduction of longevity and non-complete conversion of exhaust emissions.

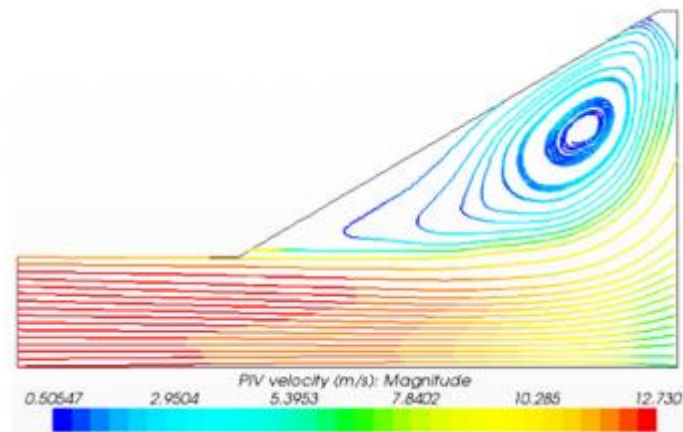


Figure 2. Velocity streamlines in the 2-D diffuser. (Porter et al. 2014)

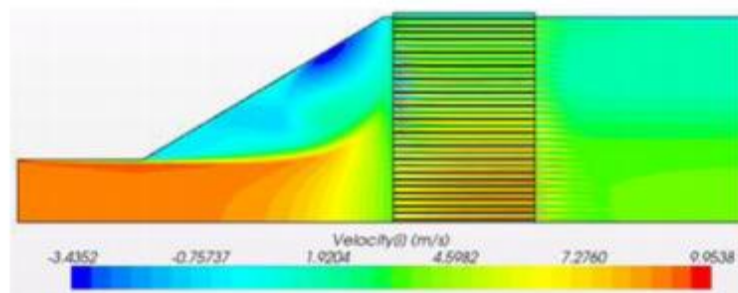


Figure 3. Velocity profile in the 2-D diffuser and monolith. (Porter et al. 2014)

Lai et al. (1991) and Kim and Son (1992) claimed the need to achieve uniform flow at the inlet of the substrate in order to achieve better performance and examined the influence of the diffuser angle on flow uniformity. The results concluded that smaller diffuser angles reduced the pressure drop within the component as well as the flow maldistribution.

Kim and Son (1999) defined a particular structure of the monolith and modified the density distribution of the channels taking into account the work done by Kaiser and Pelters (1991). They stated that lower densities, which means less number of channels per unit space, facilitated the conversion process of the gases and was more rapid, rather than high densities where there was high concentration of channels and more resistance was created to the flow. In this way, Kim et al. (1999) designed a monolith structure with higher density at the centre and lower as it approached the outer sides. The purpose with this variation of

density was to achieve a better distribution of the flow as it moved closer to the monolith centre and lower as it approached the outer sides. The purpose with this variation of density was to achieve a better distribution of the flow as it moved closer to the monolith centre.

The possibility of undertaking the analysis with Computational Fluid Dynamics tool supposed a magnificent advantage to predict the flow distribution. It became essential to define a proper and accurate model that could adjust to the configuration of the catalyst. Nevertheless it was not easy at first, as it resulted that computational fluid dynamics did not offer reliable and accurate results that could be validated. Benjamin et al. (1996) and Arias-Garcia et al. (2001) showed that this was due because it generally underestimated the degree of flow maldistribution that took place within the substrate. It took more research necessary to provide suitable analysis methods and therefore that the simulations could well match the reality.

Additionally, it can be observed in the work done by Porter et al. (2014) that there are two general approaches that can be used when analysing the component. On the one hand, the individual channel approach which consist in modelling each individual channel within the monolith. This method provided very accurate results with reasonable maximum velocities. On the other hand, the porous medium approach, which consist on assuming the monolith as porous substrate with a given resistance and permeability characteristics. It supposed a very attractive method as it provides reasonable results and also, due to its simplicity it is less computational demanding.

## 2.3. COMPUTATIONAL FLUID DYNAMICS STUDIES

To better understand the CFD basics a review of the numerical methods and governing equations of the fluid dynamics is crucial.

The fundamental equations of fluid flow dynamics stipulate the physical principles that rule the features and behaviour of any fluid. Basniev et al. (2012) and Vesteeg and Malalasekera (2007) are some examples of the numerous authors that collected and explained the numerical relations and equations of fluid mechanics. It certainly can be seen that there are three basic conservation laws that have a high relevance at this field, which are the continuity equation, the momentum equation and the energy equation.

The conservation of mass law states that matter can be changed from one form into another but the total amount of mass must remain constant. In a fluid control volume this law can be state mathematically as follows, obtaining the continuity equation:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j}(\rho u_j) = 0$$

Equation 1: Conservation of mass.

where  $\rho$  and  $u_j$  are the density and velocity component of the fluid.

The conservation of momentum law states that the momentum of a system is constant if there are no external forces acting on the system. This fundamental law is usually referred to as Newton's second law. Applying this to a fluid element we obtain the momentum equation:

$$\frac{\partial}{\partial t}(\rho u_j) + \frac{\partial}{\partial x_j}(\rho u_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \rho g_i$$

Equation 2: Conservation of momentum.

where  $\rho$ ,  $\tau_{ij}$  and  $g$  are the density, the viscous stress tensor and the gravitational acceleration respectively. There should be understood the right-hand side terms as forces acting on the fluid element while the left-hand side terms account for the rate of change of momentum and the convection of momentum.

The viscous stress tensor has been one of the great headaches for many scientists due to the difficulty of giving a simple analytical description of it. Sir George Gabriel Stokes derived a mathematical expression in 1845 for this tensor following from Newton's description of Newtonian fluids, which are those in which the viscous stresses arising from its flow are proportional to the rate of change of its deformation over time (Winklinger, 2014). This expression is as follows:

$$\tau_{ij} = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) + \lambda \frac{\partial u_k}{\partial x_k} \delta_{ij}$$

Equation 3: Viscous Stress Tensor.

where  $\mu$  is the dynamic molecular viscosity relating stresses to velocity gradients and  $\lambda$  is the bulk viscosity, which can be expressed in relation to molecular viscosity as  $\lambda = -2/3 \mu$ , that relates stresses to deformations over the fluid volume. This last statement is the central

theory of this formulation and referred to as Stoke's hypothesis (White, 1991). Furthermore the Kronecker delta, which is defined as  $\delta_{ij} = 0$  if  $i \neq j$  and  $\delta_{ij} = 1$  if  $i = j$  is used in this expression to rewrite the volumetric expansion.

Incorporating Stoke's formulation for the viscous stress tensor it is obtained the following momentum equations, also known as the Navier-Stoke's equations:

$$\frac{\partial}{\partial t}(\rho u_j) + \frac{\partial}{\partial x_j}(\rho u_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu \frac{\partial u_k}{\partial x_k} \delta_{ij} \right] + \rho g_i$$

Equation 4: Navier-Stoke's expression.

Conservation of energy law states that the total energy of an isolated system remains constant. Applied to a fluid it means that any energy exchange in a fluid element must equal to the heat change of the element and the work done on it. This fundamental law is usually referred to as the first law of thermodynamics. Applying this to a fluid element we obtain the energy equation:

$$\frac{\partial}{\partial t}(\rho h_t) + \frac{\partial}{\partial x_j}(\rho h_t u_j) + \frac{\partial p}{\partial t} + \frac{\partial}{\partial x_j}(\tau_{ij} u_i) + \frac{\partial}{\partial x_j} \left( k \frac{\partial T}{\partial x_j} \right) + S_h$$

Equation 5: Conservation of energy.

where the second right hand side term is the so-called viscous dissipation term and represents the work done on a fluid particle by surface forces. The third right hand side term is expressed in terms of Fourier's law,  $q_i = -k \frac{\delta T}{\delta x_i}$  and connects heat flow to temperature gradients. In this term thermal conductivity  $k$  acts in the same way as molecular viscosity  $\mu$  in the momentum equation. Finally, in order to be able to model a combustion system we must introduce two other minor equations that are used to close the mathematical system. Assuming gases will act as ideal gases these two equations are the thermal state equation and the caloric state equation:

$$p = \rho R T$$

Equation 6: Thermal State.

$$h = c_p T$$

Equation 7: Caloric State

In order to be able to come up with computational models that can describe physical phenomena of the flow distribution, the problem of turbulence cannot be avoided. This is due to turbulent flows being of capital importance as all relevant industrial applications make use of it. Although there does not exist an exact description of turbulence, this can be attempted by means of its known properties (Tennekes and Lumley, 1972). The most important ones are:

- Chaotic behaviour: turbulent flows have irregularity or randomness in its nature which makes a full deterministic approach very difficult. Thus, turbulent flows are usually described by means of statistical methods.
- Diffusivity: this property of turbulence boosts mixing and increases rates of momentum, heat, and mass transfer. Furthermore, turbulence becomes of increased importance in combustion processes where mixing is key due to this fundamental property.
- High Dissipation: kinetic energy gets converted into heat due to viscous shear stresses and so turbulent flows die out quickly when no energy is supplied. Energy losses occur at small turbulent scales leading to an increase of internal energy in the flow.
- Vorticity: turbulent flows are rotational; that is, they have non-zero vorticity. Therefore, mechanisms such as the stretching of three-dimensional vortices play a key role in turbulence.

Further understanding of turbulence came from Kolmogorov (1991) who first proposed a statistical approach to turbulence based on the energy cascade concept originally introduced by Richardson (1922).

Indeed, large scale eddies that originate from flow instabilities take energy from the primary flow. These eddies have a characteristic length that can be related to the main characteristic length of the problem. At these scales energy is injected into the turbulent structure. Following, these large eddies break up due to their unstable nature causing continuous energy transfer over a wide range of scales towards smaller eddies. According to Kolmogorov (1991), these kinetic energy transport phenomena is done over the inertial subrange down to the small eddies with size of the order of the Kolmogorov scale,  $\eta$ . These structures are known as the viscous subrange. Furthermore, it was also found that in the inertial subrange the spectral energy scales as  $E(k) \approx K^{-5/3}$ . This is true for any turbulent flow and is a usual value to validate numerical and experimental results regarding turbulent flows.

Given this qualitative description, there are three main approaches in order to deal with turbulence computationally. Medina et al. (2015) and Winkigler (2014) explained these methods which are the direct numeric simulation, the Reynolds averaged Navier-Stokes and large eddy simulation.

The Direct numeric simulation (DNS) method aims to, as its name suggest, and calculate all turbulent scales within any turbulent flow structure. The advantage is that there is no need of a model as the whole energy spectrum, from large energy containing structures to small dissipative eddies, will be resolves. Therefore, an extremely fine mesh able to contain all these length scales alongside with a small time step will be needed. This in turn makes this approach the one which has the most computational cost. So much so that our current computing power is unable to solve industrial problems in a reasonable amount of time, relegating this method to academic use.

The Reynolds averaged Navier-Stokes (RANS) approach, as opposed to DNS, aims to model the whole energy spectrum of a turbulent structure. This is done by solving the averaged equations in order to obtain the mean values. Thus the advantage of RANS is the low computational cost needed to solve even complex problems, which makes this method undoubtedly the most widely used CFD approach. However, the results yielded by any RANS calculation must be taken with care as they rely heavily on the turbulence model used. Although many models have stood the test of time the truth is that no universal turbulence model exists. In spite of this in many cases detailed results are not needed, making information from RANS calculations sufficient.

Large eddy simulation (LES) method can be understood as a compromise between the two aforementioned approaches. LES attempts to provide a more detailed approach than RANS calculations but still retaining valuable information by not modelling the whole range of turbulent scales. Large eddies, as its name suggests, are the ones directly calculates while the small dissipative eddies are the ones which are modelled. Furthermore, although the dissipative range is not calculated, the isotropic nature of these small eddies make model formulation much more accurate. All this enables less detailed meshes and longer time steps, which in turn reduce computational cost so that industrial application of this method is currently near viable.

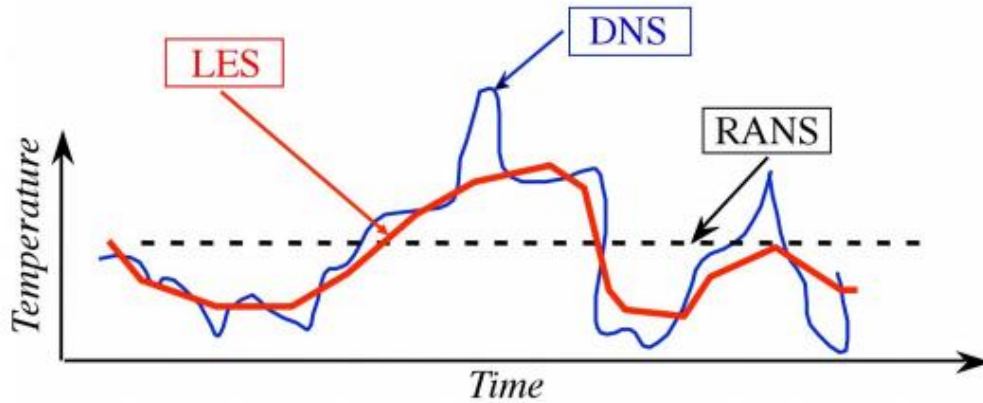


Figure 4: Representation of the expected temporal evolution of a temperature calculation using DNS, LES and RANS methods (Winkigler, 2014).

In particular, the averaging process, the governing mean equations and the closure of the system will be discussed. The averaging process, the so-called Reynolds averaging, was introduced by Osborne Reynolds in 1895. His idea was to decompose any instantaneous flow variable into its mean value and its fluctuations part (Wilcox, 1994). Therefore, the time average would be:

$$\Phi = \lim_{T \rightarrow \infty} \int_t^{t+T} \phi(t) dt$$

Equation 8: Reynolds averaging for variable  $\phi$

Where  $\phi(t) = \bar{\phi} + \phi'(t)$  as described earlier. If this concept is applied to the continuity equation Eq. 1 it can be obtained the Reynolds averaged continuity equation for compressible flow:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_j} (\bar{\rho} u_j + \overline{\rho' u_j'}) = 0$$

Equation 9: Reynolds average continuity formula for compressible flow

As we can see there is a new term  $\rho$  set of equations. The same happens with the momentum equation where we obtain three new unknowns, which generates a closure problem. This is because due to the fact that there are large temperature gradients density variations are unavoidable. The solution is to pose a density-weight average, known as Favre averaging (Favre, 1969):



$$\tilde{\Phi} = \lim_{T \rightarrow \infty} \frac{1}{T} \int_t^{t+T} \rho(t) \phi(t) dt = \overline{\frac{\rho \phi}{\rho}}$$

Equation 10: Favre averaging for variable  $\phi$

When this averaging is applied to the fundamental conservative equations it can be obtained their averaged form:

- Continuity equation:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_j} (\bar{\rho} \tilde{u}_j) = 0$$

Equation 11: Averaged continuity equation

- Momentum equation:

$$\frac{\partial}{\partial t} (\bar{\rho} \tilde{u}_j) + \frac{\partial}{\partial x_j} (\bar{\rho} \tilde{u}_i \tilde{u}_j) = - \frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j} (\bar{\tau}_{ij} - \bar{\rho} \tilde{u}_i'' \tilde{u}_j'') + \bar{\rho} g_i$$

Equation 12: Averaged momentum equation

- Energy equation:

$$\frac{\partial}{\partial t} (\bar{\rho} \tilde{h}_t) + \frac{\partial}{\partial x_j} (\bar{\rho} \tilde{h}_t \tilde{u}_j) + \frac{\partial \bar{p}}{\partial t} + \frac{\partial}{\partial x_j} \left( \alpha_{eff} \frac{\partial \tilde{h}_t}{\partial x_j} \right) + S_h$$

Equation 13: Averaged energy equation

As it can be seen, a new term  $\bar{\rho} \tilde{u}_i'' \tilde{u}_j''$  known as Reynolds stress tensor and provides six new unknowns. There exists a number of approaches in order to overcome this close problem which are reviewed below.

Launder et al. (1975) explained the Reynolds stress model (RSM). This first model aims to solve additional transport equations for the Reynolds stresses which will account for complex effects such as streamline curvature, swirl and vorticity. Due to these intricacies this method increases computational cost. Furthermore, it also suffers from stability problems which end up not justifying the use of the method.

Eddy viscosity model (EVM) was described by Versteeg and Malalasekera (2007). This widely used approach makes use of the Boussinesq hypothesis which is based on the concept of eddy viscosity. The Reynolds stresses are treated in the same way as the stresses caused by molecular viscosity and are furthermore linked to the mean rate of deformation. This eddy viscosity can be understood as the increase in viscosity due to turbulent flow.

The k-ε turbulence model was defined in the work done Jones and Launder (1972). Although this model actually is part of the EVM family its importance as an industry standard is enough to mention it. In addition to the aforementioned hypothesis, the k-ε model consists of two transport equations for the turbulent kinetic energy k and its dissipation rate ε. Its cost effective, simple and robust structure make this approach the most widely used despite its other hypothesis such as high Reynolds number and homogeneous, isotropic turbulence. The equations used for the kinetic energy and dissipation rate are:

$$\frac{\partial \bar{\rho} k}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j k}{\partial x_j} = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + P_k - \bar{\rho} \varepsilon$$

Equation 14: Modelled kinetic energy equation for k-ε model.

$$\frac{\partial \bar{\rho} \varepsilon}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j \varepsilon}{\partial x_j} = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j} \right] + C_{\varepsilon 1} \frac{\varepsilon}{k} P_k - C_{\varepsilon 2} \bar{\rho} \frac{\varepsilon^2}{k} - C_{\varepsilon 3} \bar{\rho} \varepsilon \frac{\partial \tilde{u}_j}{\partial x_j}$$

Equation 15: Modelled dissipation rate equation for k-ε model.

And the equation for modelling the eddy viscosity is:

$$\mu_t = \bar{\rho} C_\mu \frac{k^2}{\varepsilon}$$

Equation 16: Modelled eddy turbulence viscosity for k-ε model.

The latter method has been exposed by numerous researches and further information can be found in the analysis made by Launder and Spalding (1974).

Iaccarino (2001) applied the turbulence method of  $k-\varepsilon$  in conjunction with RANS model. Unfortunately, it resulted that  $k-\varepsilon$  approach was not adequate as it was not able to properly detect the flow separation at the diffuser. No acceptable results that could approximate to the real measurements were obtained.

Nevertheless, Cokljat and Kim (2003) utilised a different method known as the  $v^2 - f$  model of turbulence resulted in a good method that well-predicted the separation zone and offered reasonable results in comparison with the actual measurements of the velocity.

The model  $v^2 - f$  is based on the  $k-\varepsilon$  method and comprises an additional transport equation which enables to compute the wall-normal stress  $\bar{u}$  with respect to the walls to the walls (Durbin, 1991). In this way, the fluid could feel the interaction with the walls and the turbulence is minimized as the flow approaches to the surface by means of a damping function.

The transport equation incorporated was:

$$\frac{\partial \bar{v}^2}{\partial t} + u_i \frac{\partial \bar{v}^2}{\partial x_i} = kf - 6\bar{v}^2 \frac{\varepsilon}{k} + \frac{\partial}{\partial x_j} \left[ \left( \nu + \frac{\nu_t}{\sigma_k} \right) \frac{\partial \bar{v}^2}{\partial x_j} \right]$$

Equation 17: Expression for wall-normal stress in  $v^2 - f$  model.

Where  $\varepsilon$  and  $k$  can be obtained from the following relations:

$$\frac{\partial \varepsilon}{\partial t} + u_i \frac{\partial \varepsilon}{\partial x_i} = \frac{C_{\varepsilon 1}^* P - C_{\varepsilon 2} \varepsilon}{T} + \frac{\partial}{\partial x_j} \left[ \left( \nu + \frac{\nu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j} \right]$$

Equation 18: Modelled dissipation rate equation for  $v^2 - f$  model.

$$\frac{\partial k}{\partial t} + u_i \frac{\partial k}{\partial x_i} = P - \varepsilon + \frac{\partial}{\partial x_j} \left[ \left( \nu + \frac{\nu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right]$$

Equation 19: Modelled kinetic energy equation for  $v^2 - f$  model.

Therefore, the equation for modelling the eddy viscosity with  $v^2 - f$  model is:

$$\nu_t = C_\mu \overline{v'^2} T$$

Equation 20: Modelled eddy turbulence viscosity for  $v^2 - f$  model.

Additionally, Lien and Kalitzin (2001) proposed a modification of the original  $v^2 - f$  model that included the boundary condition of  $f=0$  at the walls.

$$k = \overline{v'^2} = f = 0, \quad \varepsilon = 2\nu k/y^2$$

Equation 21: Boundary conditions applied to  $v^2 - f$ .

As previously mentioned,  $v^2 - f$  resulted in a good method to model the motion of a fluid within a catalytic converters. Furthermore, it offered a favourable prediction of the recirculation bubbles. The turbulence intensity was good approximated, however it underestimated the kinetic energy in particular zones (Durbin, 1995).

Benjamin et al. (2001) however, focused their analysis with a different approach method. The researchers pursued the objective of achieving a proper prediction of the flow distribution that could be in accordance with experiments undertaken. They studied the behaviour of the flow as it approached the monolith channels and the deviation produced due to the resistance at the front face. They found that due to the oblique incidence of the flow to outlet channels, a significant pressure loss was produced, which needed to be taken into account in the numerical and computational methods. This phenomenon was called “the entrance effect” and its mathematical term was included in the analysis of the flow. The model approach utilised for the analysis was based on the theoretical analysis performed by Kuchemann and Weber (1953) about the flow in flat plate heat exchangers. This model is referred as  $k-w$  and it employed is for axisymmetric systems. The inclusion of the pressure term led to a better prediction of maximum velocities but it still overestimated the secondary peaks, according to the comparison with the experiments carried out with the flow rid.

Launder-Sharma model was developed also based on the standard  $k-\varepsilon$  model and incorporates a series of modifications. This model is characterised by Low-Reynolds number turbulence applications and is widely-used for solving near-wall flow behaviour. This model includes a series of damping functions which deal with the viscous and wall effects, and present the value unity away from the wall (Marthur and He, 2012).

$$\begin{aligned} & \rho \frac{\partial k}{\partial t} + \rho \frac{\partial(Uk)}{\partial x} + \frac{1}{r} \rho \frac{\partial(rVk)}{\partial r} \\ & = \frac{\partial}{\partial x} \left[ \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x} \right] + \frac{1}{r} \frac{\partial}{\partial r} \left[ r \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial r} \right] + P_k - \rho \varepsilon \end{aligned}$$

Equation 22: Modelled kinetic energy equation for Launder-Sharma model.

$$\begin{aligned} & \rho \frac{\partial \tilde{\varepsilon}}{\partial t} + \rho \frac{\partial(U\tilde{\varepsilon})}{\partial x} + \frac{1}{r} \rho \frac{\partial(rV\tilde{\varepsilon})}{\partial r} \\ & = \frac{\partial}{\partial x} \left[ \left( \mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \tilde{\varepsilon}}{\partial x} \right] + \frac{1}{r} \frac{\partial}{\partial r} \left[ r \left( \mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \tilde{\varepsilon}}{\partial r} \right] \\ & \quad + C_1 f_1 \frac{\tilde{\varepsilon}}{k} P_k - C_2 f_2 \rho \frac{\tilde{\varepsilon}^2}{k} + E_\varepsilon \end{aligned}$$

Equation 23: Modelled dissipation rate equation for Launder-Sharma model.

where

$$\tilde{\varepsilon} = (\varepsilon - D_\varepsilon).$$

And the damping functions are defined as:

$$\begin{aligned} D_\varepsilon &= 2 \frac{\mu}{\rho} \left[ \left( \frac{\partial \sqrt{k}}{\partial r} \right)^2 + \left( \frac{\partial \sqrt{k}}{\partial x} \right)^2 \right], \\ E_\varepsilon &= 2 \frac{\mu \mu_t}{\rho} \left[ \left( \frac{\partial S}{\partial r} \right)^2 + \left( \frac{\partial S}{\partial x} \right)^2 \right], \quad f_1 = 1.0, \end{aligned}$$

$$f_2 = 1 - 0.3 \exp(-Re_t^2), \quad f_\mu = \exp \left[ \frac{-3.4}{(1 + Re_t/50)^2} \right], \quad Re_t = \frac{\rho k^2}{\mu \tilde{\varepsilon}}$$

Equation 24: Modelled damping functions for Launder-Sharma model.

The k- $\omega$  model, different from k- $\varepsilon$  method, comprises transport equation for the turbulent kinetic energy k and the specific turbulence dissipation  $\omega$  (Wilcox, 1988). These terms can be obtained through the following equations:

$$\begin{aligned} & \frac{\partial}{\partial t} (\rho k) + \frac{\partial}{\partial x_j} (\rho u_j k) \\ & = \rho \tau_{ij} \frac{\partial u_i}{\partial x_j} - \beta^* \rho k \omega + \frac{\partial}{\partial x_j} \left[ \left( \mu + \sigma^* \frac{\rho k}{\omega} \right) \frac{\partial k}{\partial x_j} \right] \end{aligned}$$

Equation 25: Modelled turbulent kinetic energy for k -  $\omega$  model.

$$\begin{aligned} \frac{\partial}{\partial t}(\rho\omega) + \frac{\partial}{\partial x_j}(\rho u_j \omega) &= \alpha \frac{\omega}{k} \rho \tau_{ij} \frac{\partial u_i}{\partial x_j} - \beta \rho \omega^2 \\ &+ \sigma_d \frac{\rho}{\omega} \frac{\partial k}{\partial x_j} \frac{\partial \omega}{\partial x_j} + \frac{\partial}{\partial x_j} \left[ \left( \mu + \sigma \frac{\rho k}{\omega} \right) \frac{\partial \omega}{\partial x_j} \right] \end{aligned}$$

Equation 26: Modelled specific turbulence dissipation for k -  $\omega$  model.

with a turbulence viscosity of

$$\mu_T = \frac{\rho k}{\tilde{\omega}}, \quad \tilde{\omega} = \max \left\{ \omega, C_{\text{lim}} \sqrt{\frac{2\bar{S}_{ij}\bar{S}_{ij}}{\beta^*}} \right\}$$

Equation 27: Modelled eddy turbulence viscosity for k -  $\omega$  model.

The numerical approach was implemented in CFD with the additional pressure loss consideration and was applied by Wollin et al. (2001). The predictions were considerably improved as they minimized the difference with the experimental data at high velocities. However, with low velocity profiles the results could not provide such an accurate description, as shown in the experimental comparison made by Persoons et al. (2008).

Quadri et al. (2009) continued with the research and concluded that the correlation was not valid for very high angles of flow obliqueness and stipulated a series of correlations that were included in the CFD simulations. Liu (2003) defined a critical angle approach analysis that also improved the simulation results.

Walters and Cokljat (2008) implemented the k -  $\omega$  model by adding an additional transport equation which deals with the effects of low-frequency flow oscillations. This third equation employs the term of laminar kinetic energy  $k_l$ .

Medina and Early (2013) exposes that there exists two ways that leads to the flow transition to turbulence in the boundary layer. In case of low turbulence intensities, the transition is initiated because of the amplification of two-dimensional waves which are called Tollmien-Schlichting waves (T-S waves) (Schlichting, 1979) On the contrary, at higher turbulence intensities the T-S waves phenomena is not observed. In this case, the transition occurs due to the eddying of the stream-wise fluctuations of the fluid following the Klebanoff models (Klebanoff, 1971). The latter phenomena is known as by-pass transition and is highly related with the laminar kinetic energy concept. This concept was defined and developed by the

studies of Mayle (1991) and attempts to explain progression of high-amplitude fluctuations into by-pass transition. The increment low-frequency fluctuations is associated with the laminar kinetic energy. This is the reason why Walters and Cokljat (2008) included this term into the modelling equations.

$$k = k_{TOTAL} = k_L + k_T$$

Equation 28: Modelled total kinetic energy for  $k_t - k_l - \omega$  model.

$$\begin{aligned} \frac{Dk_T}{Dt} = & P_{k_T} + R_{BP} + R_{NAT} - \omega k_T - D_T \\ & + \frac{\partial}{\partial x_j} \left[ \nu + \frac{\alpha_T}{\sigma_k} \frac{\partial k_T}{\partial x_j} \right] \end{aligned}$$

Equation 29: Modelled turbulent kinetic energy for  $k_t - k_l - \omega$  model.

$$\frac{Dk_L}{Dt} = P_{k_L} - R_{BP} - R_{NAT} - D_L + \frac{\partial}{\partial x_j} \left[ \nu \frac{\partial k_L}{\partial x_j} \right]$$

Equation 30: Modelled laminar kinetic energy for  $k_t - k_l - \omega$  model.

$$\begin{aligned} \frac{D\omega}{Dt} = & C_{\omega 1} \frac{\omega}{k_T} P_{k_T} + \left( \frac{C_{\omega R}}{f_W} - 1 \right) \frac{\omega}{k_T} (R_{BP} + R_{NAT}) \\ & - C_{\omega 2} f_W^2 \omega^2 + C_{\omega 3} f_\omega \alpha_T f_W^2 \frac{\sqrt{k_T}}{d^3} \\ & + \frac{\partial}{\partial x_j} \left[ \left( \nu + \frac{\alpha_T}{\sigma_\omega} \right) \frac{\partial \omega}{\partial x_j} \right]. \end{aligned}$$

Equation 31: Modelled specific turbulence dissipation for  $k_t - k_l - \omega$  model.

$$\begin{aligned} \nu_{T,l} = \min \left\{ \left[ f_{\tau,l} C_{l1} \left( \frac{\Omega \lambda_{eff}^2}{\nu} \right) \sqrt{k_{T,l}} \lambda_{eff} \right. \right. \\ \left. \left. + \beta_{TS} C_{l2} Re_\Omega d^2 \Omega \right], \left[ \frac{k_L + k_{T,l}}{2S} \right] \right\} \end{aligned}$$

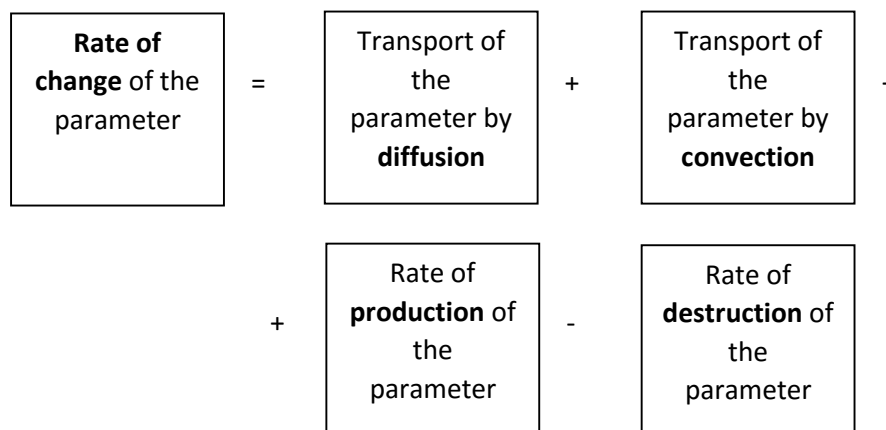
Equation 32: Modelled large eddy viscosity for  $k_t - k_l - \omega$  model.

$$\nu_{T,s} = f_W f_{INT} C_\mu \sqrt{k_{T,s}} \lambda_{eff}.$$

Equation 33: Modelled large eddy viscosity for  $k_t - k_l - \omega$  model.

Afterwards, Medina and Early (2013) developed a series of rectifications to the original model of  $k_t - k_l - \omega$  framework. This implementation included the possibility of modelling the transition in terms of surface irregularities such as backward-facing steps. Then, a novel function was proposed that included the transition sensitivity to small aft-facing steps. Applied to a flat plate with zero-pressure gradient, it was shown that this incorporation provided reasonable and good predictions.

As previously mentioned, the turbulence models aim to solve the transport equations using different parameters such as  $k, \varepsilon, k_t, k_l$  or  $\omega$  and modelled approximations. These transport equations consists of a series of terms with great significance as explained (Vesteeq and Malalasekera, 2007):



First term is referred to the variation of the variable of interest with respect to the time. For stationary parameters this term should be zero.

The second term is the diffusive contribution. Mathematically, this term is defined with a gradient and divergence and therefore proper numerical methods need to be selected to solve these operators.

The third term is the convection contribution and is represented with a divergence operator.

The final term describes the sources or sinks related to the variable of interest. Positive values of this contribution would significate a source with creation nature and negative values would be interpreted as a sink.



Different CFD programmes have been utilised along these years to carry out the simulations and provide the solutions. One of the most-commonly used was STAR-CCM by Porter et al. (2014) and Benjamin et al. (2013).

Medina et al. (2015) intended to promote the use of OpenFOAM programme and defended the main advantages that it presented. OpenFOAM is based on the finite volume method in which the computational domain is divided or discretised in small volumes. The equations and numerical relations that are computed are adapted to this finite volume approach (Moukalled et al., 1999). They highlighted its powerful utility in light design as an open source software programme with a wide range of features. The advantage of being open source makes possible the access to its usage with no need of acquiring expensive and complex programmes.

What is more, based on the assumption of porous medium by Porter et al. (2014), Medina et al. (2015) performed the simulations with OpenFOAM and compared the results of both programmes. It could be observed that both programmes predicted the same velocity flow distribution. However, both of them needed to be studied in order to improve the accuracy of the results. This can be observed in Fig. 5:

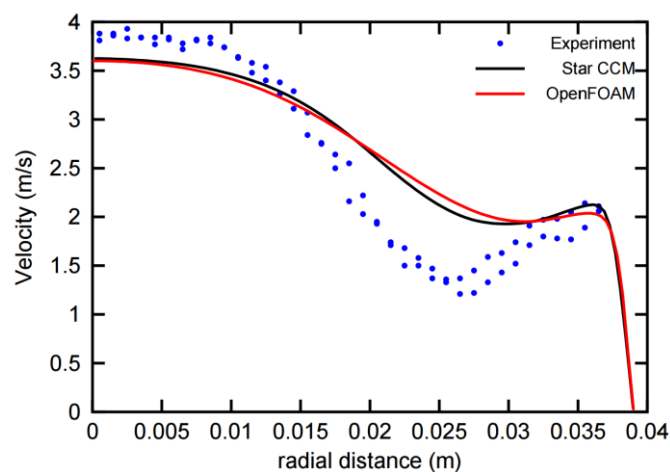


Figure 5: Downstream velocity profile (Medina, 2015).

## 2.4 CONCLUSION

It can be concluded then, that CFD has become a highly important research tool to be used in the predictions of fluid distribution. Moreover, the correct choice of the most suitable turbulence model may be critical for obtaining accurate and reliable results. Regarding the modelling of catalytic converters, RANS model is expected to be the proper method in terms of simplicity and computational cost. In the same way, turbulence models may determine the accuracy of the predictions. Despite of the lack of precision in the results with  $k-\epsilon$  model,  $v^2 - f$ ,  $k_t - k_l - w$  and Launder-Sharma seem to be adequate methods for modelling the transport equations of the flow.

## 3 CHAPTER 3. RESEARCH APPROACH

---

### 3.1 INTRODUCTION

This chapter aims to explain the research methods that are selected in order to carry out the development of the project, based on previous review of the literature. These methods must be adequate for the type of research that is intended to work out, therefore a critical selection should accurately be determined and also, a good reasoning should be provided in order to justify the choice.

### 3.2 RESEARCH METHODS

#### 3.2.1 Research process and philosophy

The research process and philosophy are general ways that allows a first approach to the research that is intended to cover. The determination of these methods should be based on a critical understanding of the topic and the different existing methodologies. The literature review allows to acquire a favourable knowledge and critical decision-making skills.

This project is characterised by an inductive method. This mechanism focuses at first on a particular situation in order to find the best reasoning and model of approach which might provide reasonable results (Godwill, 2015).

Furthermore, the projected that is intended to develop is realistic. Realism is known as an epistemological position that is usually employed in scientific research. It is independent of the human perspective and focuses on those factors which just have a single way of interpretation. Moreover, it is characterised by getting understanding of the data obtained and therefore acquiring the skills to justify its nature.

The philosophy of research which are intended to follow is the quantitative research. On the one hand, the quantitative is characterised by an objective perspective, that is, the information obtained is not judged with biased perspectives.

In the same way, the output of the research is dependant of a series of variables which influence in their final values. These factors are treated and analysed employing numerical approaches which may determine the veracity and accuracy of the results (Creswell, 2003).

It could be said then, that quantitative approach is not naturally abstract, is offers unbiased, impersonal and countable data (Bouma and Atkinson, 1995).

### 3.2.2 Research Methodology

The research methodology that is intended to be used are the numerical experiments. The numerical experiments in a type of research method within the qualitative model of research. This method includes a series of numerical equations, relations and simplifications which are performed in order to test a defined situation under some initial and boundary conditions (Srinagesh, 2006).

The numerical experiments are undertaken through a series of simulations based on the catalytic converter configuration are intended to be performed through the Computational Fluid Dynamics tool. The configuration of the component is presented as a diffuser connected to a substrate. The flow is assumed to be incompressible air, that is, with constant density and one-dimensional at the inlet of the diffuser for simplification purposes. Furthermore, the flow is analysed in a two-dimensional configuration symmetric with respect to the axis.

The CFD programme that is intended to be used to undertake the simulations is OpenFOAM within the operating system of Linux- Ubuntu.

The model of approach that is applied are the Reynolds Averaged Navier Stokes equations (RANS). In conjunction with RANS, three turbulence models are intended to be tested:

- $v^2 - f$
- $k_t - k_l - w$
- Launder-Sharma

Firstly, variations in the numerical methods for resolving the schemes of the gradient part and the divergence part within the transports equation are applied when testing  $v^2 - f$  turbulence model.

Based on the findings of the first part, the boundary conditions are modified based on the turbulence intensity and turbulence viscosity ratio magnitudes to assess the effects on the final results. The turbulence model of  $k_t - k_l - w$  is tested at this stage.

Thirdly, taking into account the best modifications and inputs which lead to higher accuracy, the turbulence model Launder-Sharma is applied and evaluated in comparison with the other two models.

Moreover, the validation of the results obtained from the simulations is necessary in order to assess their accuracy and reliability. This is achieved by benchmarked the predictions obtained from simulations against real data from real scenario. At this point, the pressure

and velocity profile and values which are computed within the catalytic monolith are examined and valuated in terms of the percentage of error that differentiate from the actual profile. The variation of the velocity within the space is the main aspect that is intended to be analysed. The programme that is going to be used for benchmark of the predictions against current results is MATLAB and its plotting tool for graphical representation. Therefore, the implementation of the models could be elaborated based on the results observed applying the necessary modifications. At the end the best model of approach is selected and additionally further work can be described based on the findings.

### 3.2.3 Data Collection

The data that is intended to be used in the project is secondary data. This type of data has is collected in an indirect way with no personal implication of the researcher. This data can have been gathered previously or can be supplied by quantitative outcomes (Caston and Katherine, 1998). The collection that is needed in order to complete this research can be obtained from different sources which are specified below.

Some examples of secondary data which is used are books, papers and thesis. These contribute to the knowledge about the background of the topic and the review of the literature, which provides a better understanding and critical vision within the field which is studied in the research.

The results obtained from simulations undertaken by Computational Fluid Dynamic tool can also be included in this categorisation. This data represents the output of the numerical experiments that are computed.

Furthermore, the experimental data which is used in order to validate the results obtained from simulations should also be pointed out. This data has been previously collected in the wind tunnel thought a series of tests.

## 4 ANALYSIS OF RESULTS

---

### 4.1 INTRODUCTION

This fourth chapter of the present work aims to presents the different results of the numerical study undergone by applying the previously described turbulence models to catalytic monolith configuration and then draw the relevant conclusions regarding model validity. The methodology and case set-up will be described to finish will the presentation and analysis of the results obtained

### 4.2 METHODOLOGY

Computational fluid dynamics (CFD) is the tool selected in order to undertake the analysis of the given configuration aimed in this project.

The actual open-source CFD software state-of-the-art includes a series of steps which are followed for its application. There can be divided in three major stages which are described below.

Pre-processing is the first stage to cover in CFD analysis. At this phase, the configuration and nature of the model which is desired to test is defined, incorporating a series of assumptions if needed. In addition, the simulation approach to the problem is selected, which is determinant in the development of the fluid mechanics equations and calculations. Based on the model of approach choice, an adequate design of the mesh configuration and suitable boundary conditions is required. The complexity and quality of the mesh can be determinant for obtaining accurate and reliable results, also considering time-consuming.

The following step is the computation stage, which characterised by the calculations fluid equations. At this point it is important the choice of the CFD programme selected to solve the fluid equations at the given configuration. It can be either commercial or open-source software.

Post-processing could the considered the final stage when applying CFD. It consists on the validation and assessment of the results obtained from the application of previous computation stage. It allows to assess the predictive capability of the software, the performance of the model and the accuracy and reliability of the results obtained.

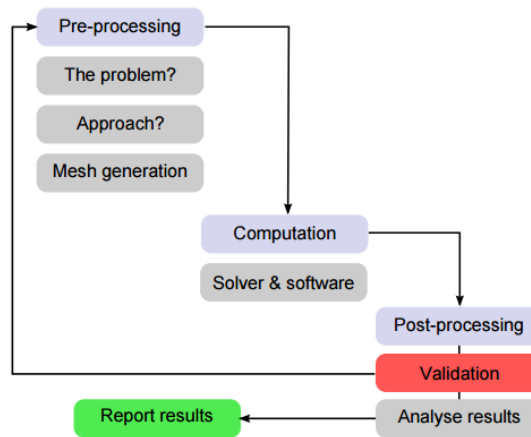


Figure 6: Typical work flow in CFD. (Medina et al. 2015)

Based on the analysis and evaluation of the outputs obtained from previously work, the case can be implemented with the aim of achieving better results or further comparison between models.

### 4.3 CASE SET-UP

This work is based on previously work introduced by Medina et al. (2015) regarding the 2D diffuser with downstream porosity. The basic configuration needed in the pre-processing step was provided and further implementations were applied.

This project aims to use OpenFOAM (3. 0. 0) CFD programme to undertake the simulations based on the configuration with the objective of determining a suitable and reliable approach.

OpenFOAM programme is an open source software, no-license is required and allows a free access to it. It also includes a collection of libraries with different functions programmed, based on the finite volume method which is characterised by the computational division of the configuration domain into smaller unit volumes. The approach models adequately adapt the computation of the equations to this space discretisation.

Moreover, one primary advantage of OpenFOAM is the easy implementation of the code and its re-usability. The availability and modifiability of the code plays an important role in the development of a suitable model that can be used to solve the given configuration.

Additionally, the programme provides a sort of useful tips via the terminal window when necessary. One benefit is that it states any problem encountered in the code and provides some suggestions to sort it out. Additionally, the user is allowed to ask for further information entering in the command the utility followed by '-help'.

All these mentioned factors contribute to the state that OpenFOAM is a suitable and competitive CFD tool for this project development.

The simulation cases in OpenFOAM basically consist on three folders where the configuration is defined and pre-processed. These three directories are required for running the computation stage, which are 0, constant and system.

In the constant directory includes the aspects that are expected to remain unchanged throughout all the simulation process. Mesh definition, transport models and turbulence model selection. It requires particular attention as the model of approach is determined here.

In this case, the modelling approach selected is RANS model because it provides suitable conditions and is not highly computational demanding. This model decomposes the flow field in fluctuating and mean values and deals with Reynolds stresses. It also deals with Reynolds stresses which are modelled using statistical information. In this way, it includes the effect of turbulence into the solutions with no complex and detailed calculations of turbulent flow field.

System folder allows the user to control the simulation and the discretisation of flow equations and also state the numerical algorithms which are used in the resolution of the flow equations. It contains three important files such as *controlDict*, *fvSchemes* and *fvSolution*.

At this part, the walls and inlet conditions are defined. It is important to highlight that the porosity nature of this project configuration is stated in *fvSolutions*. Darcy Forchheimer model is defined with permeability in the stream wise velocity.

This project intends to assess the effect of turbulence models in the solution and therefore, three models are defined and tested in *controlDict* folder. Those models are:

- $v^2 - f$
- $k_t - k_l - w$
- Launder-Sharma

```
simulationType RAS;

RAS
{
  RASModel      v2f;

  turbulence    on;

  printCoeffs   on;
}
```

Figure 7: Definition of the approach and turbulence model in OpenFOAM script.

Finally, the 0 directory includes the boundary and initial conditions, defined as text files. There should be defined the parameters required depending on the turbulence model used and the corresponding transport equations to be solved. The magnitude of those parameters may be affected by the turbulence intensity and the turbulence density ratio

stated. Consequently, both factors are modified in order to assess the influence of the input conditions in the results obtained.

Once the pre-processing data is defined the computational stage can be launched using the command `simpleFOAM`. This command is a steady-state solver for incompressible turbulent flow.

During this step, additional folders are created with the respective parameters and solved variables in each time step until a final solution converges. Some cases may not have a convergent solution so they cannot be applicable.

OpenFOAM presents post-processing tools which are really practical and useful. OpenFOAM is distributed with Paraview open source software which is aimed for results post-processing. The results obtained from previous calculations can be exported easily of several ways.

The data of the velocity variation against distance is saved in order to compare the results with the experimental data. This step allows the validation and reliability of CFD solutions and further implementation of the code.

Linux-Ubuntu operating system (OS) is selected for the installation and usage of OpenFOAM programme. This is due to the fact that Linux is the most suitable OS for running OpenFOAM and well-addresses the problems that the programme may present. OpenFOAM is distributed for Linux OS and it can be easily downloaded from its official webpage.

On the contrary, Windows operating system may not be adequate for OpenFOAM programme in terms of updated versions or code bugs.

## 4.4 RESULTS

### 4.4.1 $v^2 - f$ turbulence model

The first and second stage of the research are undertaken with the application of the  $v^2 - f$  turbulence model.

The first stage of the research aims to investigate the effect that numerical discretisation schemes for the gradient terms have on the velocity profile solution. Therefore, the script code in `fvSchemes` folder is modified and programmed for alternative methods.

```
gradSchemes
{
    default          Gauss linear;
    gradSchemeUnlimited Gauss linear;
    gradSchemeLimited cellLimited Gauss linear 1;
```

Figure 8: gradient schemes script defined for Gauss linear and cellLimited conditions

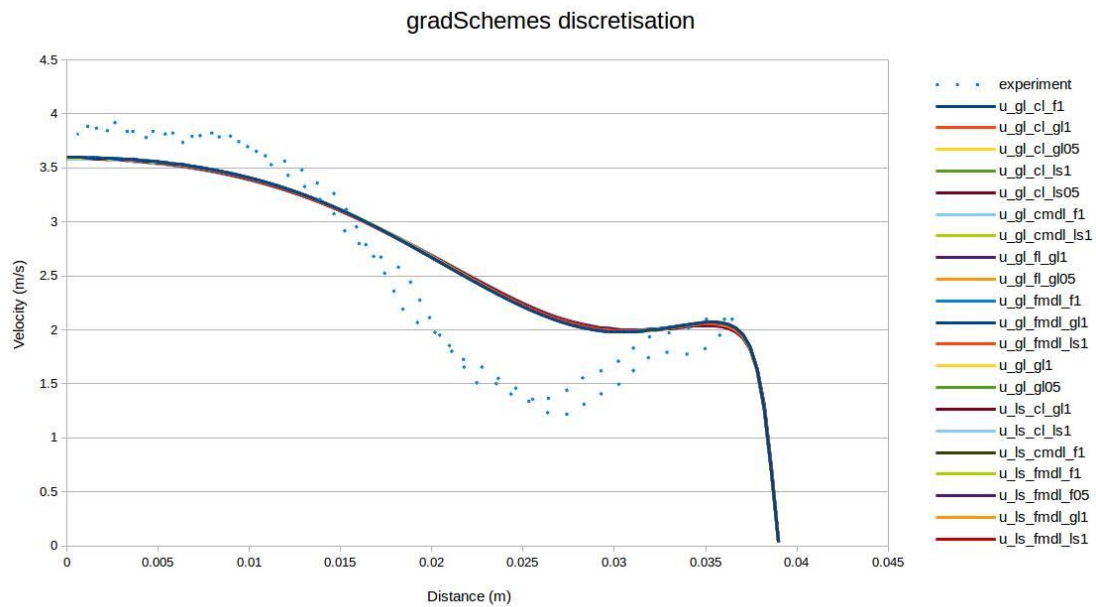


The gradSchemeUnlimited and gradSchemeLimited terms are tested for the following numerical methods:

- Gauss Linear
- Least Squares
- Fouth

Additionally, four methods employed for limiting the term gradSchemeLimited term are tested with different intensities from 0.5 to 1. These methods are:

- CellLimited
- CellMDLimited
- FaceLimited
- FaceMDLimited



Graph 1: gradient schemes numerical discretisation applying  $v^2 - f$  model

As observed in graph 1, there are not significant variations in the velocity profile for different numerical discretisation gradient schemes. Therefore, it cannot be stated any particular method that provides the best results.

The second stage of the research is to investigate the effect that numerical discretisation schemes for the divergence terms have on the velocity profile solution. Six different models were tested in conjunction with bounded Gauss method.

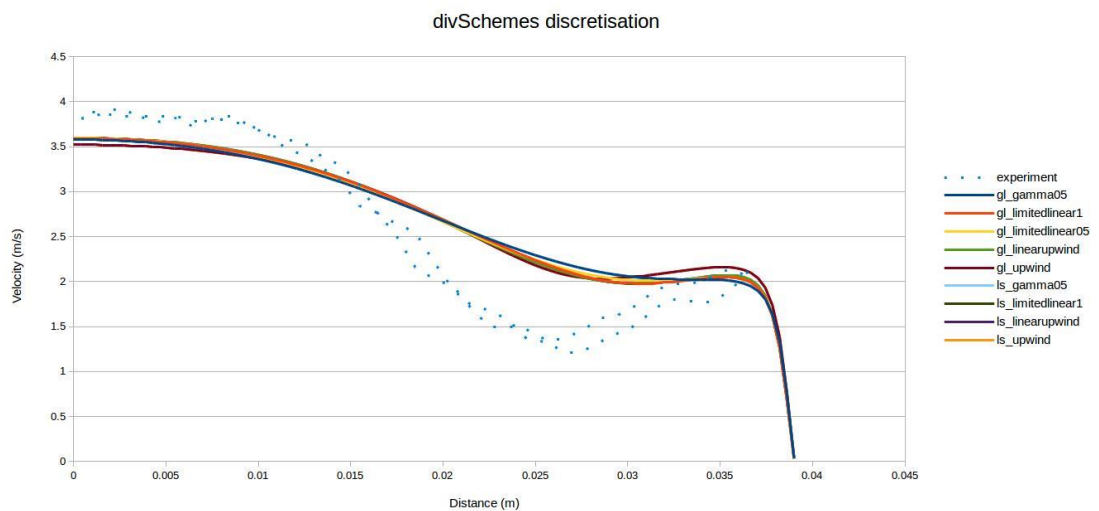
```
divSchemes
{
  default          none;
  div(phi,U)       bounded Gauss linearUpwind gradSchemeLimited;
  div(phi,k)       bounded Gauss linearUpwind gradSchemeLimited;
  div(phi,epsilon) bounded Gauss linearUpwind gradSchemeLimited;
  div(phi,nuTilda) bounded Gauss linearUpwind gradSchemeLimited;
  div(phi,omega)   bounded Gauss linearUpwind gradSchemeLimited;
  div(phi,v2)      bounded Gauss linearUpwind gradSchemeLimited;

  div((nuEff*dev(T(grad(U))))      Gauss linear;
  div((nuEff*dev2(T(grad(U))))     Gauss linear;
}
```

Figure 10: divergence schemes script defined for Gauss linear and linearUpwind conditions

The methods applied at this stage were the following:

- Upwind
- Linear upwind
- Quick
- Gamma
- LimitedLinear
- Superbee



Graph 2: divergence schemes numerical discretisation applying  $v^2 - f$  model

In graph 2, It could be observed higher variation in the results when modifying the divergence terms compared to the gradient terms. However, no determinant approximations to the experimental solution was achieved.

The most suitable method taking into account the trends in the velocity profile is the linear Upwind discretisation using Gauss Linear. Neither superbee nor quick method provided solutions to this configuration.

#### 4.4.2 $k_t - k_l - \omega$ turbulence model

The third stage of the research is developed using a different turbulence model, the  $k_t - k_l - \omega$  and Gauss linear Upwind method for the divergence schemes discretisation.

This stage is characterised by the modification of the input conditions in the catalytic configuration, based on the variation of two parameters which are the turbulence intensity and eddy viscosity ratio. The magnitude of these two influential parameters has a direct effect in the variation of the input conditions which can be quantified by means of the transport equations.

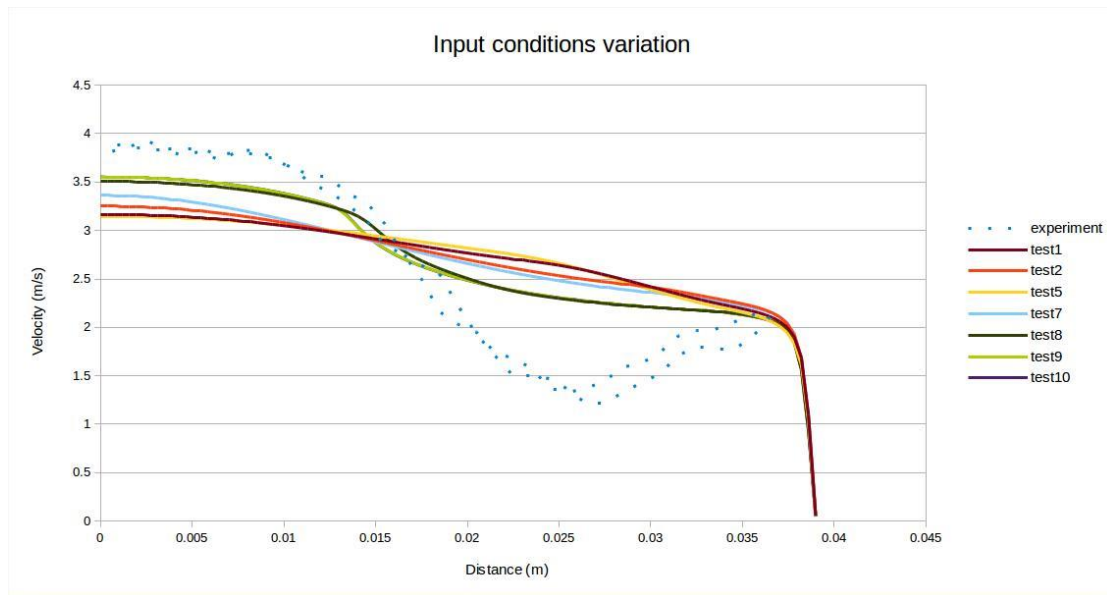
Depending on the turbulence model which is used, the computation of results requires different input conditions which are applied in the corresponding transport equations. In this case, it is necessary to define the magnitude of  $k_t$ ,  $k_l$  and  $\omega$ .

Ten different tests were run and plotted against experimental data with the following values:

	Turbulence Intensity	Eddy viscosity ratio
Test 1	0,01	10
Test 2	0,1	10
Test 3	0,005	10
Test 4	0,01	50
Test 5	0,01	5
Test 6	0,005	50
Test 7	0,1	5
Test 8	0,5	5
Test 9	0,1	1
Test 10	0,5	1

Table 1: Input conditions for  $k_t - k_l - \omega$  tests.

Higher variation on the velocity profile can be observed in graph 3. This allows to dismiss certain approaches and to focus in the most determinant and influential input conditions. In this case, it can be observed that last test presented higher similarity to the experimental data.

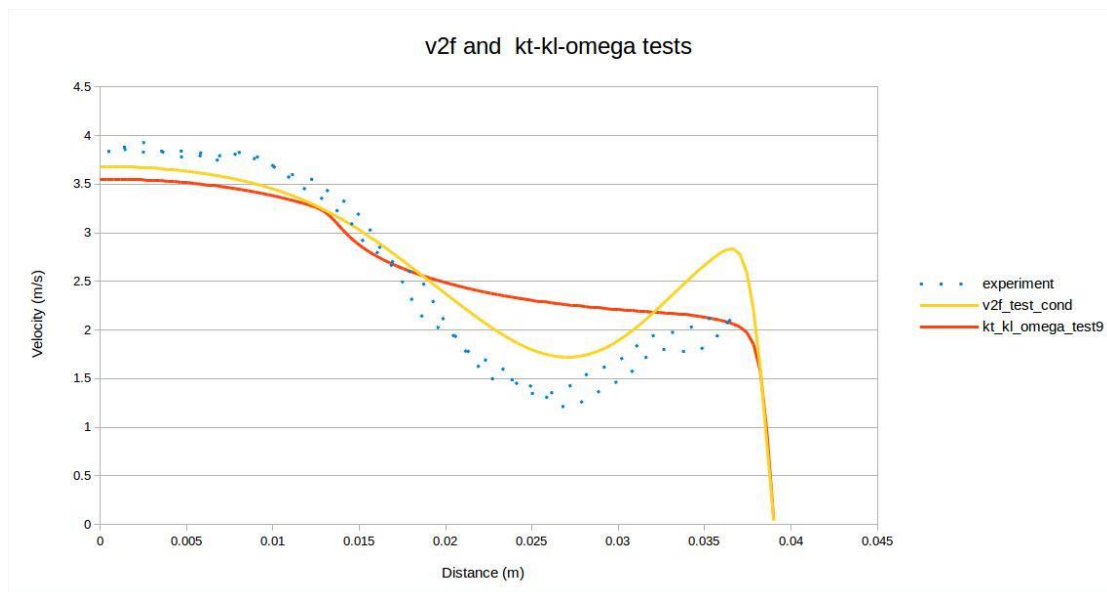


Graph 3:  $k_t - k_l - \omega$  tests with different input conditions

It should be mentioned that tests which are not plotted do not provide a converged result. Also, Test 9 and Test 10 plots presented a similar solution.

However, when  $k_t - k_l - \omega$  is compared to  $v^2 - f$  turbulence model it can be observed less accuracy in the results, with flatter trends in the velocity profile. Therefore,  $v^2 - f$  model was applied taking into account the findings of this stage and varying the input conditions. In order to test this model is necessary to state the basic conditions of  $K$ ,  $\epsilon$  and  $v^2$  based on test 9 values for turbulence intensity and eddy viscosity ratio.

The results obtained when  $v^2 - f$  model was applied reflected a better approximation to the experimental case, with more similarity in the velocity trends.



Graph 4:  $k_t - k_l - \omega$  and  $v^2 - f$  tests with the same input conditions

### 4.4.3 Launder-Sharma turbulence model

In this stage, Launder-Sharma model is defined and tested based on the most suitable parameters magnitudes and numerical methods tested in previous research. Hence, two tests are undertaken.

Linear UpWind is the numerical method for the discretisation of the divergence schemes as previously defended.

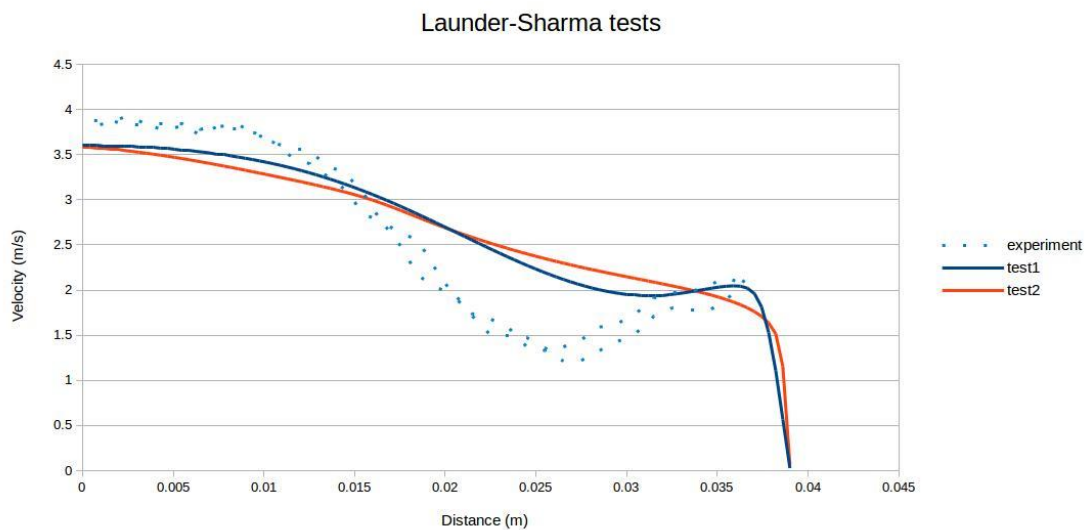
Test 1	
Turbulence Intensity	Eddy viscosity ratio
0,01	10

Table 2: Input conditions for  $v^2 - f$  test1.

Test 2	
Turbulence Intensity	Eddy Viscosity ratio
0,1	1

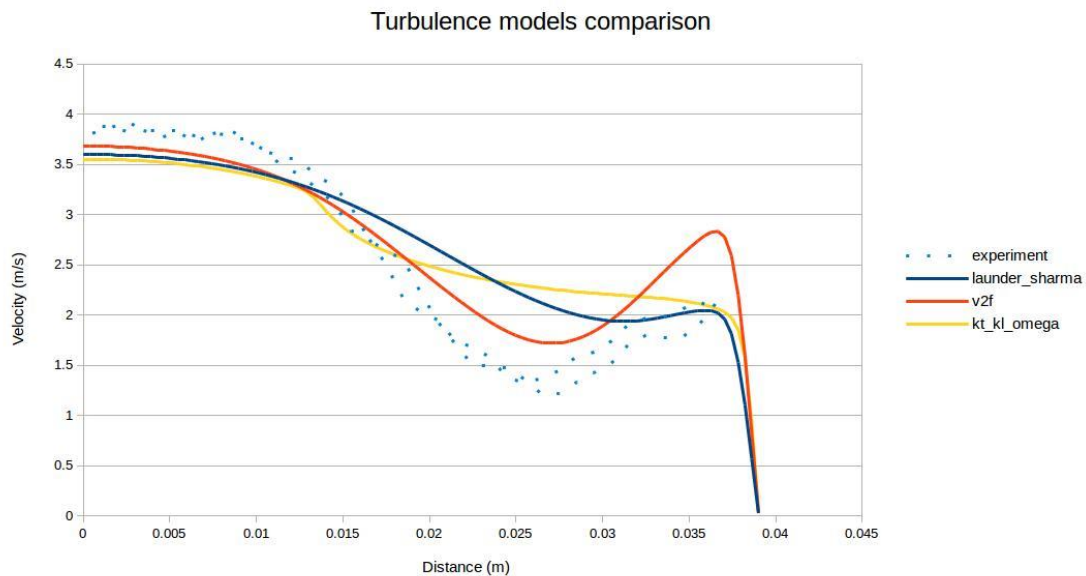
Table 3: Input conditions for  $v^2 - f$  test 2.

As a result, the first test provides better velocity solutions:



Graph 5: Launder-Sharma tests with the two different conditions

Finally, Launder-Sharma best solutions are compared to previous turbulence models  $v^2 - f$  and  $k_t - k_l - \omega$  as shown in graph 6.



Graph 6:  $v^2 - f$ ,  $k_t - k_l - \omega$  and Launder-Sharma tests with the same conditions

As observed,  $k_t - k_l - \omega$  results to offer the less satisfactory solutions with flatter velocity trends when compared to experimental data. It is followed by Launder-Sharma model, which provides better results and proper trends. However, it is observed that  $v^2 - f$  is the model which presents the best velocity profile solution and have higher similarity with respect to the experimental profile.

## 4.5 CONCLUSION

It could be concluded that  $v^2 - f$  model is presented as the most suitable turbulence model in conjunction with RANS approach to predict the flow distribution in the given catalytic configuration. Nevertheless,  $k_t - k_l - \omega$  model resulted in less accurate velocity trends when compared to experimental data.

The effect of numerical schemes discretisation of gradient terms is not determinant in the final solution.

On the other hand, the numerical schemes discretisation of divergence terms presented higher variations and upwind model was stated to an adequate method.

Finally, the most suitable input conditions resulted to be 0,1 for turbulence intensity and 1 for eddy viscosity ratio.

## 5 CONCLUSION AND RECOMMENDATIONS

---

This chapter aims to provide a critical overview of the work development and the achievement of the project aims. Furthermore, it is presented a summary of the process and the most relevant findings in each stage related to the set objectives of this project.

Further work and recommendations are suggested based on the results obtained and the work direction.

### 5.1 CONCLUSION

This project aimed to assess the performance of the different turbulence models in a defined catalytic monolith configuration. For that end, RANS was the primary model of approach selected based on its suitable balance between reliable results and consumption of time. Additionally, the three different models  $v^2 - f$ , Launder-Sharma, and  $k_t - k_l - \omega$  were applied and tested.

Three main questions were attempted to be answered:

- How does the choice of discretisation scheme affect the CFD results provided by the  $v^2 - f$  model?
- How accurate are state-of-the-art RANS models in predicting the flow within an idealised catalytic converter (benchmarked against experimental data)?
- Will a transition-capable RANS model ( $k_t - k_l - \omega$ ) lead to improved CFD predictions?

Using  $v^2 - f$  turbulence model, it was examined the effect that numerical discretisation schemes for the gradient terms had on the velocity profile solution. However, no substantial change was observed in the results that could be considered determinant.

Additionally, it was investigated the effect of the numerical discretisation schemes for the divergence terms. The solutions resulted in higher perceived changes in the velocity profile with respect to the previous tests and allowed to state the Linear upWind method as the proper one.

Using  $k_t - k_l - \omega$  turbulence model, the input conditions were modified based on the variation of two influential parameters; the turbulence intensity and the turbulence viscosity ratio. The result provided more significant variations in the velocity profile and proper approximation to the experimental data could be achieved. Nevertheless, it was observed that this model provided flatter velocity trends with respect to previous  $v^2 - f$  turbulence model and furthermore did not correspond to the actual trends. Therefore, based on the findings, the most suitable input conditions were applied using the  $v^2 - f$  model.

Finally, the Launder-Sharma turbulence model was tested with the proper numerical schemes discretisation and parameters of test 1 and test 2 from previous stage. The first test showed better results than the second one, the opposite to  $v^2 - f$  model.

It can be observed that Launder-Sharma provided better solutions than  $k_t - k_l - \omega$  turbulence model. However,  $v^2 - f$  model still remains to be the best model when results are benchmarked against the experimental data.

It can be concluded then, that  $v^2 - f$  is presented as the most adequate turbulence model compared to  $k_t - k_l - \omega$  and Launder-Sharma for this catalytic monolith configuration and RANS approach. The gradient terms no presented significant influence. The divergence term which shows to be is upwind with Gauss-linear numerical method. The input conditions present determinant effect in the velocity profile, based on the values of 0,1 for turbulence intensity and 1 for eddy viscosity ratio.

Nevertheless, further research should be undertaken in order to investigate better approximations to the experimental data.

## 5.2 FURTHER WORK AND RECOMMENDATIONS

Future research about this topic should be developed in order to achieve a better approximation to the experimental results.

It could be observed that the modification of boundary and initial conditions provided a determinant change in the velocity profile with respect to the distance. Therefore, it would be interesting to pay particular attention in the proper definition of these parameters that could well adjust to the actual case.

Additionally, further research could be made regarding the implementation of the turbulence models applied and to assess the limitations of RANS approach.



## LIST OF REFERENCES

---

- Arias-García, A., Benjamin, S.F., Zhao, H. and Farr, S. (2001) *A comparison of steady, pulsating flow measurements and CFD simulations in close coupled catalysts*. No. 2001-01-3662. SAE.
- Basniev, K. S., Dmitriev, M. N., Chilingar, G. V., Gorfunkle, M., Nejad, A. G. M. (2012) *Mechanics of fluid flow*. Winley: Hoboken.
- Becker, E. R. and Zygourakis, K. (1987) "Design options for rapid light-off of monolith catalytic converters." *Journal of Industrial and Engineering Chemistry*.
- Benjamin, S.F., Clarkson, R.J., Haimad, N. and Girgis, N.S. (1996) *An experimental and predictive study of the flow field in axisymmetric automotive exhaust catalyst systems*. No. 961208. SAE
- Benjamin, S.F., Haimad, N., Roberts, C.A and Wollin, J. (2001) "Modelling the flow distribution through automotive catalytic converters. Proceedings of the Institution of Mechanical Engineers" *Journal of Mechanical Engineering Science*, 215 (4): 379-383.
- Bouma, G. and Atkinson, J. (1995) *A handbook of social science research* Oxford University Press: Oxford.
- Cho Y-S., Kim D-S., Han M. H. et al. (1998) *Flow distribution in a close-coupled catalytic converter*. No. 982552. SAE.
- Clarkson, R. J. (1995) *A Theoretical and Experimental Study of Automotive Catalytic Converters*. Unpublished Ph.D. thesis. Coventry: Coventry University.
- Comfort, E. H. (1974) "Monolithic catalytic converter performance as a function of flow distribution" *ASME Winter Annual Meeting*, Paper No. 74-WA/HT-30.
- Creswell, J. (2003) *Research design: qualitative, quantitative, and mixed methods approaches* Sage: London

- Durbin, P. (1991) "Near-wall turbulence closure modeling without damping functions." *Theoretical and Computational Fluid Dynamics*, 3 :1–13.
- Durbin, P. A. (1995) "Separated flow computations with the k- $\epsilon$ -u<sup>2</sup> model" *AIAA Journal*, 33 (4): 659-664.
- Favre A. (1969) *Statistical equations of turbulent gases in problems of hydrodynamics and continuum mechanics*. SIAM: Philadelphia.
- Godwill, E. A. (2015) *Fundamentals of Research Methodology. A Holistic Guide for Research Completion, Management, Validation and Ethics* Nova Science Publishers: Hauppauge.
- Hagevik, G. H. (1970) *Decision making in air pollution control*. Paeger: London.
- Haimad, N. (1997) *A Theoretical and Experimental Investigation of the Flow Performance of Automotive Catalytic Converters*. Unpublished Ph.D. thesis. Coventry: Coventry University.
- Heck, R. H., Wei, J. and Katzer, J. R. (1976) "Mathematical modelling of monolithic catalysts." *AIChE Journal* 22 (3), 447-484.
- Howitt, J.S. and Sekella, T. C. (1974) *Flow Effects in Monolithic Honeycomb Automotive Catalytic Converters*. No. 740244. SAE.
- Iaccarino, G. (2001) "Predictions of turbulent separated flow using commercial CFD codes" *ASME Journal of Fluids Engineering*, 123(4): 819-828.
- Jones W. P. and Launder B. E. (1972) "The prediction of linearization with a two-equation model of turbulence." *International Journal of Heat and Mass Transfer*, 15: 301–314.
- Kaiser, F. W. and Pelters, S. (1991) *Comparison of metal-supported catalysts with different cell geometries*, No: 910837, SAE.
- Kim, J. Y. and Son, S. (1999) *Improving Flow Efficiency of a Catalytic Converter Using the Concept of Radially Variable Cell Density-Part I*. No 1999-01- 0769. SAE.

Klebanoff, P. (1971) "Effects of free-stream turbulence on a laminar boundary layer" *Bull. Amer. Phys. Soc.* 10: 1323.

Kolmogorov A. N. (1991) "The Local Structure of Turbulence in Incompressible Viscous Fluid for Very Large Reynolds Numbers." *Proc. R. Soc. London*, 434: 9–13.

Kuchemann, D. and Weber, J. (1953) *Aerodynamics of Propulsion*. McGraw-Hill: New York.

Lai M.-C., Kim J. Y., Cheng C.-Y. et al. (1991) *Three-dimensional simulations of automotive catalytic converter internal flow*. No. 910200. SAE.

Liu, Z., Benjamin, S.F. and Roberts, C.A., (2003) Pulsating flow maldistribution within an axisymmetric catalytic converter-flow rig experiment and transient CFD simulation. SAE 2003-01-3070, SP-1801 SAE International Warrendale, PA.

Liu, Z. (2003) *Pulsating flow maldistribution in automotive exhaust catalysts; Numerical modelling and experimental correlation*. Unpublished Ph.D thesis. Coventry: Coventry University.

Launder, B. E., Reece, G. J. and Rodi, W. (1975) "Progress in the Development of a Reynolds-Stress Turbulence Closure." *ASME Journal of Fluids Engineering* 68: 537–566.

Launder B. E. and Spalding D. B. (1974) "The Numerical Computation of Turbulent Flows." *Computer Methods in Applied Mechanics and Engineering.*, Vol. 3, pp. 269–289, 1974.

Lemme, S.J. and Givens, W.R. (1974) Flow through catalytic converters – An analytical and experimental treatment. No. 740243. SAE.

Lien, F. S. and Kalitzin, G. (2001) "Computations of transonic flow with the v2f turbulence model." *International Journal of Heat and Fluid Flow*, 22(1):53–61.

Mayle, R. E. (1991) "Role of laminar-turbulent transition in gas turbine engines" *American Society of Mechanical Engineers* 113 (4): 509–536.

Medina, H. and Early, J. (2013) "Modelling transition due to backward-facing steps using the laminar kinetic energy concept". *European Journal of Mechanics – B/Fluids*, 4: 60-68.

- Medina, H. J., Beecham, A., Saul, J. , Porter, S. , Aleksandrova, S. and Benjamin, S. (2015) 'Open source Computational Fluid Dynamics using OpenFOAM' , 'Light Aircraft Design: Methods and Tools'. Held 16 November 2015 at Royal Aeronautical Society: London.
- Mathur, A., He, S. (2012) Performance and Implementation of the Launder-Sharma Low-Reynolds number turbulence model.
- Moukalled, F., Mangani, D. and Darwish M. (2015) "The Finite Volume Method in Computational Fluid Dynamics." *Springer International Publishing*.
- Patel, B. and Patel, K. (2012). "A Review Paper on Catalytic Converter for Automotive Exhaust Emission." *International Journal of Applied Engineering Research* 7: 1398-1402.
- Pelters S., Kaiser F. W. and Mauss W. (1989) The development and application of a metal supported catalyst for Porsche's 911 Carrera 4. No 890488. SAE International Journal of Engines.
- Persoons, T., Vanierschot, M, Van den Bulck, E., (2008) "Oblique inlet pressure loss for swirling flow entering catalyst substrate". *Experimental Thermal and Fluid Science* volume 32, 1223-1231.
- Porter, S., Mat Yamin, A.K., Aleksandrova, S., Benjamin, S.F., Roberts, C.A. and Saul, J. (2014) "An assessment of CFD applied to steady flow in a planar diffuser upstream of an automotive catalyst." *SAE International Journal of Engines* 7 (4): 1697-1704.
- Quadri, S., Benjamin, S.F. and Roberts, C.A. (2009) "An experimental investigation of oblique entry pressure losses in automotive catalytic converters. Proceedings of the Institution of Mechanical Engineers" *Journal of Mechanical Engineering Science*, 223 (11): 2561-2569.
- Richardson L. F. (1922) *Weather Prediction by Numerical Process*. Cambridge University Press: Cambridge
- Searles, P.S., Flint, S.D., Diaz, S.B., Rousseaux, M.C., Ballare, C.L., Caldwell, M.M. (2002) "Plant responses to solar Ultraviolet-B radiation in a southern South American Sphagnum peatland". *Journal of Ecology* 90: 704-713.

Schweich, D. and Leclerc, J. P. (1990) *Flow, heat and mass transfer in a monolithic catalytic converter*. '2nd International Conference on Catalysts and Automotive Pollution Control' held in September 1990. Brussels.

Shah, R.K. (1978) "A correlation for laminar hydrodynamic entry length solutions for circular and noncircular ducts" *ASME Journal of Fluids Engineering* 100.

Srinagesh, K. (2011) *The Principles of Experimental Research* Elsevier Science: Burlington.

Tennekes, H. and Lumley, J. L. (1972) *A first course in turbulence*. MIT Press: MIT.

Versteeg, H. K. and Malalasekera, W. (2007) *An introduction to computational fluid dynamics: the finite volume method*. Harlow: Pearson Prentice Hall.

Walters, D. and Cokljat, D. (2008) "A three-equation eddy-viscosity model for Reynolds averaged navier-stokes simulations of transitional flow" *ASME Journal of Fluids Engineering* 130 (12): 1–14.

Weltens, H., Bressler, H., Terres, F., Neumaier, H., Rammoser, D., (1993). *Optimization of catalytic converter gas flow distribution by CFD predictions*. No. 930780. SAE.

White F. M. (1991) *Viscous Fluid Flow*. McGraw-Hill: Rhode Island.

Wilcox D. C. (1994) *Turbulence Modeling for CFD*. DCW Industries, La Cañada.

Wilcox, D. C. (1993) *Turbulence Modeling for CFD*. DCW Industries: La Cañada.

Winklinger (2014) *Implementation of a combustion model based on the flamelet concept and its application to turbulent reactive sprays*. Unpublished Thesis. Valencia: Polytechnic University of Valencia.

Wollin, J. and Benjamin, S.F. (1999) *A study of the flow performance of ceramic contoured substrates for automotive exhaust catalyst systems*. No. 1999-01-3626. SAE.

Wollin, J. (2001) *A study of Pulsating Flow in Automotive Exhaust Catalyst Systems*, Unpublished Thesis. Coventry: Coventry University.

Yamin, A.K.M. (2012) *Pulsating flow studies in a planar wide-angled diffuser upstream of automotive catalyst monoliths*. Unpublished Thesis. Coventry: Coventry University.

Zygourakis, K., (1989) "Transient operation of monolith catalytic converters: a two-dimensional reactor and the effects of radially non-uniform flow distributions." *Chemical Engineering Science* 44 (9) 2075-2086.

## APPENDIX I –PROJECT MANAGEMENT

---

### Introduction

The aim of this document is to reflect the project management to provide an updated Gantt Chart where all the main stages are presented and time-measured. Additionally, the problems encountered during the project development are explained and the decisions related to the solutions to sort them out are stated.

The project stages could be divided in the following parts:

- Introduction to the project
- Study of  $v^2 - f$  turbulence model.
- Study of  $k_t - k_l - w$  turbulence model
- Study of Launder – Sharma turbulence model
- Elaboration of the report

The time-management was based on an estimation of effort and dedication required for developing each stage.

Furthermore, the main tool used to undertake this project is OpenFOAM 3.0, based on Computational Fluid Dynamics (CFD) analysis.

This programme has better performance when using Linux-Ubuntu Operating System as it represents the major distributor and well-addresses the problems that may arise. Therefore, the installation of this operating system had to be made in the personal laptop.

In order not to remove Windows operating system a disk partition was made, defining 80 Mega Bytes for Linux. The version of Linux chosen was Ubuntu 15.10.

The disk partition was not easy at first and further research was needed to be made in order to be documented of the steps to follow. Meanwhile, in order to make progress within the project and the simulations it was important to make a decision to find a temporal solution. Then, a virtual machine was installed in Windows 7 which allowed to operate in Linux-Ubuntu operating system with no need of partition. This choice could not be used in future simulations because of its computing limitations and low performance. Additionally, an external disk was needed to move all the existing data in the laptop.

The installation of the programme was needed to be done again in the proper operating system.

## Development of the project

### Introduction to the project

The first step was to define the aim and objectives of the project. This part is determinant in the direction that the project is willing to follow and the performance.

Once the aims and objectives were established, it was necessary to get engaged with Computational Fluid Dynamics (CFD) and OpenFOAM programme. In order to obtain knowledge in the basic commands and functionality of the programme, a series of tutorials were covered using the website and downloaded OpenFOAM package. This step was really important to get engaged with the tools and also command window of Linux.

### Study of $\nu^2 - f$ study model

This was the model presented in most of the simulation tests. Due to this fact, the simulations were prevised to last more time compared with the rest of models of study.

### Study of $k_t - k_l - w$ turbulence model

The application of this model implied the calculation of the input boundary conditions based on the variation of certain parameters. This part allowed to gain understanding in the application of the equations to define the input conditions. To do so, simplified equations were needed to be found and solved for certain parameters values.

### Study of Launder-Sharma turbulence model

This model was used just to assess the comparison with the rest of models and state the proper one. Unfortunately, there was difficult to obtain detailed information about this model. Some papers were asked online but no answers were received.

The application and simulations of Launder-Sharma model took less time compared to the previous models.

## 5.3 ELABORATION OF THE REPORT

The report was elaborated with two different deadlines. The first, was on the 12<sup>th</sup> of February for introduction, research methods and literature review chapter. This deadline was set according to the interim review submission point.

Subsequently, the analysis of results and conclusion and recommendations chapter was finished by the 25<sup>th</sup> of April. This second part needed to have sufficient results obtained from the simulations in order to be elaborated.

## Additional Problems

The personal laptop suddenly stopped working because of fails in the mother board. This was critical for the project development due to the high dependence on the software to run the calculations. This fact supposed a temporal standstill of the work done by the software. A new laptop was required and bought. Meanwhile all this time was dedicated to the report preparation, writing and implementing the chapters.

Linux-Ubuntu operating system had to be installed in the new laptop using a partition with Windows 10. In the same way, Open FOAM programme had to be installed. The installation was easy and fast at this point.



## The interim review

An interim review was performed at half of the module duration. At this time, certain work was needed to be completed.

In terms of report elaboration, the introduction, the literature review and the research methods chapters were fully completed.

In terms of the simulations, many  $v^2 - f$  simulations and numerical discretisation study was completed and post-processed.

## Meetings

Frequent meetings with the supervisor were appointed to review the state of the project and to ensure the proper direction of the work. Weekly meetings since November were attended with the usual structure as follows:

Part one: This part focused in the current progress and project issues.

- Review of the student and project progress
- Review of the work done by the student and feedback provided by the supervisor
- Discussion about the challenges encountered and actions taken to overcome them.
- Analysis of the results obtained.
- Student questions or doubts about this points asked and answered by the supervisor.

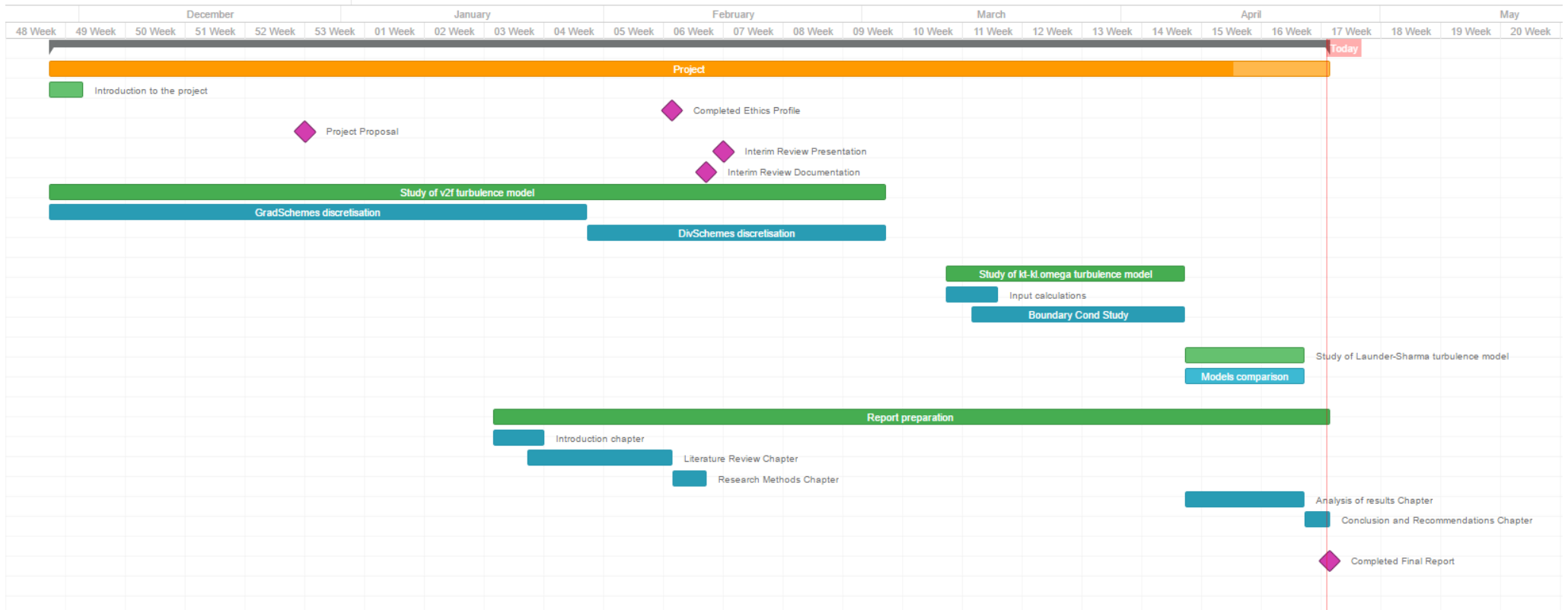
Part two: This second part focused in the agreed key action points taken regarding the project development.

- To discuss about the implementation of the work that has been done.
- To agree the next steps to take.
- To set-up the deadlines or update them if needed
- To discuss about the project direction and management and future work to do.
- Student question or doubts about this points asked and answered by the supervisor.

## Conclusion

The main purpose of the project was completed on time in terms of computational simulations, post-processing of results and report elaboration. The project stages can be mainly divided in five different parts with the corresponding demands and implications. Meanwhile, a series of problems such as the installation of Linux Operating System, laptop crash or certain wrong code definitions were encountered. Consequently, decisions were taken to find adequate solutions, time. Profit and adapt the project management to the actual situation.

# Gantt Chart



## APPENDIX II – PROJECT PROPOSAL

---

# Final Year Undergraduate Project Proposal Form

Student Name	Nour Sanchez Abad
Course	None - Erasmus Student
Email	sanchezn@uni.coventry.ac.uk
Project Module	320EKM

Supervisor	Humberto Medina
------------	-----------------

**Project Title:**

*A proposed title for the project (Should be meaningful, relevant and concise)*

Numerical study of the predictive capabilities of Reynolds Averaged Navier-Stokes (RANS) turbulence models applied to catalytic converters

**Synopsis:**

*Explain the background to the project, and provide an overview of what you intend to do (approximately 500 words)*

Air pollution is a constantly growing concern that industry and organisations need to face nowadays. It has been demonstrated that one of the major factors that contributes to the level of the air pollution comes from the automotive sector. Engines produce a sort of toxic emissions to the atmosphere such as carbon monoxide (CO), unburned hydrocarbons (HC) and oxides of nitrogen (NOx). These gases are harmful and affect to people's health and to the environment. Due to this reason, emission regulations started to be defined and imposed by the institutions. As a response to the raised claim, the industry developed new types of devices to reduce the emissions.

This project deals with the analysis of one of these components that is the catalytic monolith using the method of Computational Fluid Dynamics and a further benchmark of the results

obtained against the experimental data.

Computational Fluid Dynamics (CFD) is a tool which is widely used in the industry as well as in the investigation sector to analyse the flow behavior through a component with a defined configuration under determined initial and boundary conditions with a selected computational model of approach. The main purpose is to recreate a desired scenario represented by the set-up conditions and to check the performance of the component. The computational fluid Dynamics programme that will be used to the project development is OpenFOAM within Linux operating system.

Furthermore, the computational model of approach which will be applied are the Reynolds-averaged Navier-Stokes equations (RANS). This model provides an averaged solution which is based on mean and fluctuating factors, aspect that represents a limitation that needs to be considered. Additionally to this model, turbulence approach models will applied and the solutions will be tested by means of OpenFOAM simulations.

Several simulations will be undertaken so that it could be examined the effect that common numerical discretisation schemes for the gradient and the divergence term of the turbulence models have on the solution obtained within RANS. This will be observed in the changes of the pressure and velocity distribution over the space and time.

The monolith component is usually located after a diffuser and composed by a series of channels within which chemical reactions take place in order to reduce the toxicity of the exhaust gases. Nevertheless an ideal configuration of an ideal monolith will be used to perform the analysis in order to simplify the calculations and computational process. Despite of the fact that simplifications are assumed, the configuration selected is still a good representation of the real one. It includes a 2-dimensional diffuser, a porous medium which acts as the monolith and one outlet region. The flow maldistribution will be tested at the latter part of the configuration and will be compared with the result obtained from experiments. Flow behavior is important because the efficiency of the system will depend on the profile distribution.

Finally, MATLAB numerical computing programme will be used to benchmark the CFD results against the experimental data and to validate the most suitable CFD model in terms of accuracy and computing performance.

**Client:**

*Provide a description of your client (if any), and contact details.*

Not applicable.

--

This project will provide a better understanding of the predictive capability of selected RANS models to capture the flow physics. The configuration analysed is usually present in catalytic monoliths. As result, the key beneficiaries from this project will include automotive engineers who use CFD to design these products, but also the automotive industry in general. Since an understanding of the accuracy of turbulence models is important to help improve produce design, performance and facilitate their development.

**Objectives (provide from 5 to 8):** *List the overall objectives of the project. These should be measurable, and will be used to assess the level of achievement of the project.*

- To carry out a literature review to appraise the state-of-the-art in relation to CFD applied to emission after-treatment devices.
  - To gain a solid understanding of the assumptions behind RANS modelling and 3 target turbulence models.
  - To investigate the effect that common numerical discretisation schemes for the gradient terms of the turbulence models have on the numerical solution.
  - To investigate the effect that selected upwind numerical discretisation schemes for the divergence terms of the turbulence models have on the numerical solution.
  - To evaluate at least 3 low Reynolds RANS models applied to an idealised catalyst configuration.
  - To critically analyse and evaluate the results obtained and compare them with the experimental data. The variation of pressure and velocity will be examined.
  - To write a detailed technical report to communicate the key findings from this work.

**Project Deliverables (provide from 5 to 8):**

*Provide a list of key deliverables of the project (which may be one for each of the above objectives). These can be studies, reports, recommendations, etc.*

- Choice of the proper analysis models to be tested based on the literature review information.
- Performance of computational fluid dynamics simulations and numerical computation through OpenFOAM and MATLAB programmes.
- A qualitative assessment of the effect that grad. Schemes have on the results obtained from CFD simulations.
- A qualitative assessment of the effect that div. Schemes have on the results obtained from CFD simulations.
  - A critical appraisal of 3 RANS models and detailed differences that can be observed in the simulations performance and results.
- A detailed technical report which explains the most suitable model to be used taking into account the research outputs and the comparison with the experimental data.

**Why are you interested in the project?**

*Provide a reason for your interest, and describe what greater general interest it serves. Who else could benefit from it?*

This project is presented as a challenge to all my years of study within the Engineering field. It is the opportunity to apply the academic knowledge, critical perspective and soft skills that I have been acquiring at university. It also forms part of my learning process as there are many new aspects that I have never worked with such as the application of analysis models. The computational fluid dynamics is a very important method of analysis that highly contributes to all engineering student experience. It is also widely used in the Industry sector as well as in investigation. Therefore, it not only contribute to your personal development but also to future professional life.

Moreover, this project is that the progress made could still be implemented and improved with further research. It also could be used as part or basis of a more significant analysis.

Another reason why I am willing to undertake this project is because I find that the possible applications related with exhaust emissions is one of the most important issues that is needed to be investigated nowadays. The sustainability and green-impact is a real concern that requires focused research because of people and environment care.

**What are the key questions the project attempts to answer (provide from 1-3)?**

- How does the choice of discretisation scheme affect the CFD results provided by the v2f model?
- How accurate are state-of-the-art RANS models in predicting the flow within an idealised catalytic converter (benchmarked against experimental data)?
- Will a transition-capable RANS model (k-kl-omega) lead to improved CFD predictions?

**How will you judge whether your project has been a success?**

The project will be judged with a critical analysis and understanding of the results obtained through the different simulations using OpenFOAM and MATLAB programmes. The acquisition of these skills will facilitate the determination of the best approximation model. Moreover, a comparison with the experimental data will be needed in order to ensure that the results match with the real case.

**What research methods do you intend to use?**

The methodology that is intended to be used are simulation performed by Computational Fluid Dynamics and numerical computing. Furthermore, the main modelling approach which is intended to be used is RANS model.

Simulation results will be benchmarked against the experimental data in order to assess the accuracy of the simulation as well as to validate the model and numerical setup such as scheme choice.

All the process will be covered using OpenFOAM and MATLAB programmes.

**What primary and/or secondary data sources do you intend to use?**

No primary data is intended to be used.

Secondary data sources which are intended to be used are;

- Experimental data
- Books
- Scientific Articles
- Papers
- Dissertations
- PhD Thesis
- Internet

**Estimate the number of hours you expect to spend on each of the major project tasks:**

*(The tasks below are only examples. You will need to edit the table to suit your own project).*

Introduction	10
Objectives	30
Literature Review	50
Case Studies	60
Research	30
Final report preparation	20
Total number of hours	200

Signature: Nour Sanchez Abad

Date: 25/01/2016

## APPENDIX III - ETHICS APPROVAL CERTIFICATE

---





## **Certificate of Ethical Approval**

Applicant:

Nour Sanchez Abad

Project Title:

Numerical study of the predictive capabilities of Reynolds Averaged Navier-Stokes (RANS) turbulence models applied to catalytic converters.

This is to certify that the above named applicant has completed the Coventry University Ethical Approval process and their project has been confirmed and approved as Low Risk

Date of approval:

25 February 2016

Project Reference Number:

P41274

## APPENDIX IV – LOG BOOK

---

## Face-To-Face Student/Supervisor Meeting Record

Project Title:	Numerical Study of the predictive capabilities of RANS turbulence models applied to catalytic converters		
Student Name:	Nour Sanchez Abad	Student ID:	6744065
Supervisor:	Humberto Medina	Student UID:	
Supervisor UID:		School:	MAA
Course Code:	NONE - ERASMUS STUDENT	Module Code:	
Date Today:	27/11/2015	Time:	09.30h.

**Current Progress and Issues:***(Include challenges encountered and actions taken to overcome them)*

- Introduction to the topic, installation of software (Linux - Ubuntu) and programme (OpenFOAM).
- Main data and results provided.

**Agreed Key Action Points:***(Include dates of any deadlines)*

- To complete the installation of Linux and disk partition. (December)
- To read through OpenFOAM userguide and tutorials

**Date and Time of next meeting:**

04/12/2015

Signatures of those present:

**Supervisor:****Student:**


## Face-To-Face Student/Supervisor Meeting Record

Project Title:	Numerical Study of the predictive capabilities of RANS turbulence models		
Student Name:	Nour Sanchez Abad	Student ID:	6744065
Supervisor:	Humberto Medina	Student UID:	
Supervisor UID:		School:	MAA
Course Code:	NONE - ERASMUS STUDENT	Module Code:	
Date Today:	04/12/2015	Time:	09.30h.

applied  
to  
analytic  
concepts

**Current Progress and Issues:**

(Include challenges encountered and actions taken to overcome them)

- Explanation of the case
- Discussion of possible applications

**Agreed Key Action Points:**

(Include dates of any deadlines)

- To focus in the variation of velocity and the graph  $u_x$  vs. distance.
- To modify the numerical methods for the calculations, plot the results, and try to adjust the graph.

**Date and Time of next meeting:**

11/12/2015

Signatures of those present:

**Supervisor:**

**Student:**



## Face-To-Face Student/Supervisor Meeting Record

Project Title:	Numerical Study of the predictive capabilities of RANS turbulence models applied to catalytic converters		
Student Name:	Nour Sanchez Abad	Student ID:	6744065
Supervisor:	Humberto Medina	Student UID:	
Supervisor UID:		School:	MAA
Course Code:	NONE - ERASMUS STUDENT	Module Code:	
Date Today:	11/12/2015	Time:	09:30

**Current Progress and Issues:***(Include challenges encountered and actions taken to overcome them)*

- Problems with plots in matlab using data from paraFoam graphs.  
↓
- Explained and resolved. Example with one of the cases. using 'Octave'!

**Agreed Key Action Points:***(Include dates of any deadlines)*

- To continue working and plot the graphs in matlab in order to compare them.

**Date and Time of next meeting:**

22/01/2016

Signatures of those present:

Supervisor:

Student:



## Face-To-Face Student/Supervisor Meeting Record

<b>Project Title:</b>	Numerical Study of the predictive capabilities of RANS turbulence models applied to catalytic converters		
<b>Student Name:</b>	Nour Saad & Abad	<b>Student ID:</b>	6744065
<b>Supervisor:</b>	Humberto Medina	<b>Student UID:</b>	
<b>Supervisor UID:</b>		<b>School:</b>	MAA
<b>Course Code:</b>	NAME-ERASMUS student	<b>Module Code:</b>	
<b>Date Today:</b>	22/01/2016	<b>Time:</b>	10:00h.

**Current Progress and Issues:**

*(Include challenges encountered and actions taken to overcome them)*

v2f model

- Changes made in Grad Schemes → Grad Schemes Limited.  
 Cell Limited / Cell MD Limited / Face Limited / Face MD Limited / ~~Face MD~~ and  
 Gauss Linear / Least Squares / fourth 1/0.5  
 → Grad Schemes Unlimited Gauss Linear / Least Squares
- Total of 60 tests carried out. Not all of them gave a convergent result.  
 • Plotted the results in matlab → Similarities between the results <sup>showed</sup>

**Agreed Key Action Points:**

*(Include dates of any deadlines)*

- Changes in Grad Schemes → Default + Grad Schemes Limited. Use the same approximation in both of them; Cell limited Gauss Linear x, cell MD limited Gauss Linear x, face limited Gauss Linear x, face MD limited Gauss Linear x, Gauss Linear x. (Total of 5 tests)
- Changes in Div Schemes → to be determined
- Turbulence Models → to be determined

**Date and Time of next meeting:** 29/01/2016

Signatures of those present:

**Supervisor:**

**Student:**



## Face-To-Face Student/Supervisor Meeting Record

Project Title:	Numerical Study of the predictive capabilities of RANS turbulence models applied to catalytic converters		
Student Name:	Nour Sanchez Abad	Student ID:	6744 CCS
Supervisor:	Humberto Medina	Student UID:	
Supervisor UID:		School:	MAA
Course Code:	NONE-ERASMUS student	Module Code:	
Date Today:	29/01/2016	Time:	10:30h.

**Current Progress and Issues:***(Include challenges encountered and actions taken to overcome them)*

- Calculations run in Openfoam with the changes in Grad Schemes. Cannot be plotted in Matlab because of a problem with windows (Blue Screen showed)
- Project Proposal Form delivered

**Agreed Key Action Points:***(Include dates of any deadlines)*

- To plot the results obtained from Grad Schemes tests.
- To undertake the tests in with ~~Grad~~ Div Schemes changes
- To read about v2f and k-k<sub>ε</sub>-ω turbulence models
- To arrange a meeting for next week.

**Date and Time of next meeting:**

05/02/2016

Signatures of those present:

Supervisor:

Student:



## Face-To-Face Student/Supervisor Meeting Record

Project Title:	Numerical study of the predictive capabilities of RANS turbulence models		applied to catalytic converters
Student Name:	Nour Sanchez Abad	Student ID:	6744065
Supervisor:	Humberto Medina	Student UID:	
Supervisor UID:		School:	MAA
Course Code:	NAWE - ERASMUS Student	Module Code:	
Date Today:	05/02/2016	Time:	10:00h.

**Current Progress and Issues:***(Include challenges encountered and actions taken to overcome them)*

- Problems with laptop: it stopped working. It cannot be repaired, important components (such as the motherboard) need to be changed with new ones → New Laptop
- Interim Review and documents. Deadline: 12/02/2016.  
Including: Gantt charts, chapters (Introduction, Research Methods and literature review) and log-book.  
Presentation will be held the week after.

**Agreed Key Action Points:***(Include dates of any deadlines)*

- To complete the ~~the~~ Interim Review Documentation.
- Overview of the contents within the Chapters

**Date and Time of next meeting:**

12/02/2016

Signatures of those present:

**Supervisor:****Student:**




**Face-To-Face Student/Supervisor Meeting Record**

<b>Project Title:</b>	Numerical Study of the predictive capabilities of RANS turbulence models	<b>Student ID:</b>	6744065
<b>Student Name:</b>	Nour Sánchez Abad	<b>Student UID:</b>	
<b>Supervisor:</b>	Humberto Medina	<b>School:</b>	MAA
<b>Supervisor UID:</b>		<b>Module Code:</b>	
<b>Course Code:</b>	NONE - ERASMUS student	<b>Time:</b>	10:00
<b>Date Today:</b>	12/12/2015		

models applied to catalytic converter

**Current Progress and Issues:**

*(Include challenges encountered and actions taken to overcome them)*

- Interim review: draft chapters of the Introduction, Literature Review and Research Methods.
- Gantt chart elaboration

**Agreed Key Action Points:**

*(Include dates of any deadlines)*

- ~~To~~ To implement the literature review with a more focused description of transport equations and the schemes.
- To implement the research methods
- To elaborate the Interim Review Presentation
- To test the div Schemes in U2F model of turbulence

**Date and Time of next meeting:**

19/02/2016

Signatures of those present:

Supervisor:



Student:

**Face-To-Face Student/Supervisor Meeting Record**

<b>Project Title:</b>	Numerical Study of the predictive capabilities of RANS turbulence models applied to catalytic converters		
<b>Student Name:</b>	Nour Sanchez Abad	<b>Student ID:</b>	6744065
<b>Supervisor:</b>	Humberto Medina	<b>Student UID:</b>	
<b>Supervisor UID:</b>		<b>School:</b>	MAA
<b>Course Code:</b>		<b>Module Code:</b>	
<b>Date Today:</b>	19/02/2016	<b>Time:</b>	10:00h.

**Current Progress and Issues:**  
*(Include challenges encountered and actions taken to overcome them)*

- Interim Review Presentation
- Interim Documentation Uploaded {
  - Introduction draft
  - Research methods draft
  - Literature review draft
  - Logbook
  - Gantt chart
- Reading about the schemes

**Agreed Key Action Points:**  
*(Include dates of any deadlines)*

- Test
- To test div Schemes (v2f model) with different numerical methods such as:
  - Upwind
  - Gamma
  - Linearwind
  - Limited Linear
  - Superbee
  - Quick
- Review of the literature about the Div Schemes.

**Date and Time of next meeting:** 26 / 02 / 2016

Signatures of those present:

Supervisor:

Student:



## Face-To-Face Student/Supervisor Meeting Record

<b>Project Title:</b>	Numerical study of the predictive capabilities of RANS turbulence models		
<b>Student Name:</b>	Nour Sanchez Abad	<b>Student ID:</b>	6744065
<b>Supervisor:</b>	Humberto Medina	<b>Student UID:</b>	
<b>Supervisor UID:</b>		<b>School:</b>	MAA
<b>Course Code:</b>		<b>Module Code:</b>	
<b>Date Today:</b>	18/03/2016	<b>Time:</b>	10.00h.

to apply  
to convert

### Current Progress and Issues:

(Include challenges encountered and actions taken to overcome them)

- To change the turbulence model employed in the simulations →  $k-\epsilon-w$
- To identify the variables that are needed to be defined at the initial conditions
- To search for the corresponding equations to determine the value of these variables
- Problem with the simplification of the equations

### Agreed Key Action Points:

(Include dates of any deadlines)

- Solved the problem with the simplification of the definitions
- To try to test the models applying the adequate definitions at the initial conditions

**Date and Time of next meeting:** 25/03/2016

Signatures of those present:

Supervisor:

Student:



## Face-To-Face Student/Supervisor Meeting Record

<b>Project Title:</b>	Numerical study of the predictive capabilities of RANS turbulence models applied to		
<b>Student Name:</b>	Nour Sánchez Abad	<b>Student ID:</b>	6744065
<b>Supervisor:</b>	Humberto Medina	<b>Student UID:</b>	
<b>Supervisor UID:</b>		<b>School:</b>	MAA
<b>Course Code:</b>		<b>Module Code:</b>	
<b>Date Today:</b>	11/03/2016	<b>Time:</b>	10.00h.

catalyst  
convert

<b>Current Progress and issues:</b> (Include challenges encountered and actions taken to overcome them)	
<p>Div Schemes tested in u2f model. Solution provided with: Upwind, Gamma 0.5, Linear Upwind, Limited Linear.</p> <p>Failed: Gamma 1, Quick, Spalart</p> <p>All the results were plotted and benchmarked against the experimental data. → Wrong data used.</p>	
<b>Agreed Key Action Points:</b> (Include dates of any deadlines)	
<p>To change the experimental data plot and use the correct values.</p> <p>To change the plot design (lines, points...)</p> <p>To start testing other models → <math>k_f k_w</math> and Launder-Sharma.</p>	
<b>Date and Time of next meeting:</b>	16.00h. 11/03/2016

Signatures of those present:

Supervisor:

Student:

