CFD Modelling of Generic Gas Turbine Combustor

Master’s Thesis in Solid and Fluid Mechanics

AMIR KHODABANDEH

Department of Applied Mechanics
Division of Fluid Dynamics
CHALMERS UNIVERSITY OF TECHNOLOGY
Göteborg, Sweden 2011
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ABSTRACT

New computational methods are continuously developed in order to solve problems in different engineering fields. One of these fields is gas turbines, where the challenge is to make gas turbines more efficient and to reduce emissions that are bad for the environment. One of the main parts of a gas turbine that can be improved is the combustion chamber. In order to optimize the combustion chamber, both experimental and numerical methods are called for. Numerical optimization implies the necessity to model the most important phenomena in combustion chambers such as turbulent swirling flow, chemical reactions, heat transfer, and so on. In this project we try to design a simple yet accurate model, for a generic combustor of industrial interest, that may be tested in a relatively short time and that yields reliable results. An important topic is here to perform grid sensitivity studies to make sure that the model yields mesh independent results. Another topic of interest is the choice of turbulence model and how this choice affects the grid sensitivity. Heat transfer models are also important to evaluate. Different turbulence models and heat transfer models done with this generic geometry and results will be discussed. After this project we made a model that is numerically reliable, mesh independent and fast.

Key words:
Computational Fluid Dynamics, CFD, Gas turbine, Combustion chamber, Grid study, Convection, Conduction.
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Preface

In this study, numerical simulation of generic gas turbine combustor chamber has been studied. The study has been carried out from August 2010 to September 2011. The project is carried out at the department of Applied Mechanics, division of Fluid dynamics, Chalmers University of Technology, Sweden. The thesis was done under supervision of Lic. Eng. Abdallah Abou-Taouk and Professor Lars-Erik Eriksson. All the calculations have been carried out at C3SE, Chalmers Centre for Computational Science and Engineering, Chalmers University of Technology, Sweden.

Foremost, I would like to express my sincere gratitude to my supervisors Prof. Lars Erik Eriksson and Lic. Eng. Abdallah Abou-Taouk for the continuous support of my Master thesis, for their patience, motivations, enthusiasm, immense knowledge and their valuable feedbacks on the report. Their guidance helped during the research and writing of this thesis. I could not have imagined having this thesis finished without their support.

My deepest gratitude goes to my family for their unflagging love and support throughout my life; this dissertation is simply impossible without them. I am indebted to my father, Hamid agho, for his care and love. I cannot ask for more from my mother, maman Janet, as she is simply perfect. I have no suitable word that can fully describe her everlasting love to me. I feel proud of my big brother, Khosrow kako, for his talents. He had been a role model for me to follow unconsciously when I was a teenager and has always been one of my best counsellors.

Göteborg September 2011

Amir Khodabandeh
Notations and abbreviations

Roman upper case letters
$C_{1\varepsilon}$ First constant in $\varepsilon$ equation
$C_{2\varepsilon}$ Second constant in $\varepsilon$ equation
CFD Computational Fluid Dynamics
$D$ Diffusion coefficient
$F_i$ Force vector ($i^{th}$ component)
$\text{NOx}$ generic term for the mono-nitrogen oxides NO and NO2
$S_{ij}$ Strain rate tensor

Roman lower case letters
$c$ Concentration
$h$ Convective heat transfer coefficient
$k$ Turbulence kinetic energy
$t$ time
$u$ Velocity vector

Greek upper case letters
$\phi$ Blend factor

Greek lower case letters
$\beta^*$ Constant in k- $\omega$ model
$\partial_j \frac{\partial}{\partial x_j}$
$\varepsilon$ Dissipation of turbulent kinetic energy
$\sigma_{ij}$ Cauchy stress tensor
$\rho$ Density
$\theta_T$ Kinematic eddy viscosity
$\omega$ Specific dissipation
1 Introduction

1.1 Gas turbine

Energy is needed in order to make machines work. One of the best forms of energy is electrical energy. It can be carried over distances and can be produced almost anywhere with proper tools. There are several devices that produce electrical energy such as solar panels, wind turbines and gas turbines. In this project we will focus on gas turbines. Gas turbines produce electrical energy from burning a combustible mixture of fuel (e.g. natural gas or evaporated hydrocarbons) and air. When the gas mixture burns, the volume of the gas will increase. This expansion in gas volume makes a rotor of a turbine rotate and this rotation may then be converted to electrical energy.

There are two important families of gas turbines:

1-Stationary gas turbines: this type of turbine is used to produce power in large scales, for example in power plants.

2-Turbofan and turbojet gas turbines: these turbines are used usually as aero engines, and are sometimes referred to as jet engines. A variety of turbofan and turbojet gas turbines are used in military and commercial aircraft.
1.2 Gas turbine components

Stationary and turbofan gas turbines are based on the same thermodynamic cycle; the Brayton cycle. Therefore they have many similarities in terms of structure. The schematic picture below shows common parts:

![Figure 3. Schematic of gas turbine](p3)

These parts are:

Inlet: A gas turbine can have one or several inlets, based on their design and usage. Inlets are used to send fuel and air into the gas turbine. The main inlet in front of the gas turbine is used to suck air in; while there are several other small inlets existing further downstream in order to inject fuel.

Compressor: Compressors are used to increase the pressure of the inlet air, in order to increase the efficiency of the turbine. The effect of compressor, as well as other parts, can be described by using Brayton cycle, as shown in the Figure A2. The area that enclosed between the points 1,2,3,4,1 in the PV diagram, shows the net work output of the cycle. In the Figure A2, the process that took place between point 1 and point 2 is the compressor effect; it will raise pressure from point 1 to point 2. From the diagram one can expect that output work will rise with the raise of pressure in the point 2. On the other hand pressure at point 2 is limited by several parameters such as material constraints, temperature raise and etc.

Combustor: Here, fuel is mixed with the air and then burns. This reaction results in increasing temperature and volume. Volumetric expansion can drive the rotor blades of a turbine or a turbojet to produce work or thrust. This is an isobaric process. In Figure A2, this process is between points 2 and 3.

Turbine: Its job is to drive the compressor shaft and, in the case of a stationary gas turbine, to provide useful mechanical work to drive for example an electrical generator. In ideal cycle, this process is isentropic.

Outlet: This section is designed based on gas turbine usage; for stationary gas turbine the outlet is a low speed exhaust, which will guide combustion products out of system, either to the environment or to other cycles. For the turbofan gas turbine the outlet is a jet nozzle, which will increase velocity to produce thrust.
1.3 Combustion Chamber

The combustion chamber is the place where two major events take place; at the inlet fuel will mix completely, or to a sufficient degree, with air. In some combustors fuel mixes with air before combustors, however, in order to achieve a smooth burning, air and fuel should be mixed before burning. Depends on when fuel will mixes with air, combustors divided in to two groups that will be discussed later in this chapter. Second event is burning. In the combustion chamber, due to the high temperature, the gaseous mixture which consists of fuel and air will ignite and raise the temperature. Rise in temperature will increase the volume which will drive the fluid forward.

There are number of facts that make this part of gas turbine important.

In order to make this clear, we will address problems in a poorly designed combustion chamber. There are several problems that can occur:

1- Poor mixing: When fuel is not mixed enough with air, it can burn incompletely which results in increased levels of CO, soot, NOx and unburned hydrocarbons (UHC).
2- Uneven combustion: This happens when temperature of a section goes high but the neighbouring sections are colder, thus this can result in extra thermal stresses. Thermal stresses may in time lead to material fatigue and failure.
3- Environment: incompletely burned gases or unburned hydrocarbons (UHC) can poison the environment. UHC, NOx and soot are important factors for each burning device. The design should lower them as much as possible.
4- Economy: With increasing price of oil, it is important that gas turbines have high efficiency and therefore low fuel consumption. One of the most important parts, in order to achieve high efficiency, is the combustion chamber.

Above factors shows the importance of combustion chambers in gas turbines.

There are two types of combustors, diffusion flame combustors and premixed combustors. In diffusion flame combustors, fuel and air mixing and combustion takes place simultaneously. Speed of flame is limited by the rate of diffusion. These kinds of combustors are simple to build and operate, but they are not environmentally clean. The major drawback of these combustors is that the flame exists mainly at stochiometric conditions. This can result in high rates of NOx production.

The other type of combustor is premixed flame combustors. These combustors are newer than the diffusion flame combustors. They mix the fuel with air to a high degree thus the flame exists where the fuel exists, if it can be stabilized. Contrary to the previous combustor type these combustors are more complex and harder to design, but they produce less NOx. Every day new challenges arise for gas turbines. Different factors like increase in oil price, new type of fuels like bio fuels, different design like premix combustors and many other factors will challenge engineers to develop new combustors or improve the existing combustors. These challenges require new tools. One of the important tools that can help engineers is numerical modelling or in other words CFD.
2 Thesis description

2.1 Aim of project

- The main focus of this project is to do a grid study for a characteristic gas turbine combustion chamber.
- Using different turbulence models on a characteristic gas turbine combustion chamber.
- Modelling the convective and conductive heat transfer of the casing with the ambient.

2.2 Software

In this project three software packages were used.

1- ICEMCFD: This software is used to draw the surface geometry. Then it used again in order to mesh the computational domain which is bounded by the surface geometry.

2- CFX: This is the solver software. This software is used to simulate the flow in the computational domain. Also some part of the post processing is carried with CFXpost

3- Matlab: It is used together with CFXpost to post process the results, plot charts etc.

2.3 Limitation

The time frame of this project was 1 year, so the chosen geometry could not be too complex (further detail on this part will be discussed on geometry section). Calculations took place on the local Linux cluster BEDA, with 8 processors. Each simulation needed about 9 days of wall clock time.

The design of geometry was done on a desktop computer. Due to the limited project time the grid generation work had to be minimized and therefore the combustor geometry had to be simplified.
3 Calculation methodology
3.1 Geometry Simplifications

The simplifications that were done are the following:

- The most common combustors have no symmetry in the domain usually coming from the locations of the burner inlets. The first simplification was to omit these inlets so the geometry becomes symmetric. This implied that only $45^\circ \left(\frac{1}{8}\right)$ of the full geometry were modelled, shown in Figure 4.

![Figure 4. This is one section that has been modelled.](image)

- We assume one inlet for the fuel and the air. The most common combustors have separate inlets for fuel and air. Both the fuel and the air are assumed to be perfectly mixed at the inlet.
- NOx formation was neglected and assumed that the fuel will be burn completely.

![Figure 5. Modelled geometry](image)
The simplified geometry consists of an inlet, a guide vane and an outlet. Top and bottom faces are set to walls, while the side faces are axial symmetric ones. This is shown in Figure 5.

There is a secondary inlet in the CFD-domain, named ignition inlet. This inlet is used in the beginning of the iteration process to ignite the fuel. When the flow has ignited the mass flow rate is set to zero.

The full geometry is shown in Figure 6, which consists of 8 sectors.

![Figure 6. Full modelled geometry](image)

### 3.2 Grid generation

Four different mesh sizes were investigated in the present work. These consist of 400,000 or 400K, 500,000 or 500K, 1,000,000 or 1M and 2,000,000 or 2M cells. Each section consists of a vane, which is shown in Figure 7.

![Figure 7. Three section of geometry.](image)

In Figure 7, three sections are shown. In Figure 7, some part of wall is in different colour with the name of “Free slip wall” or “ramp”. This section name separately from other walls, because of strange interaction of k-ω model, this section should be free slip wall contrary to other walls.
Figure 8 shows the grid and parts that were difficult to mesh. Vane was the hardest part to mesh. On the front face the vane cut top wall and thus, as it is shown in Figure 8, it is not on one plane.

The trailing edge of the vane is shown in Figure 9. We just flat the V shape trailing edge in order to raise the mesh quality. If V shape edge were used, as it is in reality, mesh quality in this case drops significantly.
The wall in front of the vane was raised in order to obtain higher quality of the grid. This wall is illustrated in Figure 10. This modification is so small that their effect on the flow field can be neglected.

Figure 10. Vane interaction with wall

3.3 Boundary conditions

Boundaries locations’ have been shown in the Figure 5. Boundary conditions are as follow unless otherwise stated:

- Inlet: \( \text{CH}_4 \) mass fraction: 0.039494, \( \text{O}_2 \) mass fraction 0.22570, Mass flow rate: 0.00625 Kg/s, Turbulence: Low Intensity and Eddy Viscosity Ratio.
- Outlet: Opening, Pressure: 1 atm, Temperature: 300K
- Walls: Adiabatic and free slip
- Reference pressure: 0 atm
- Combustion Extinction Temperature: 750 K
- Domain is rotational periodic

3.4 Governing equations

It exists six equations that should be solved to model the flow field. These equations are continuity, momentum, energy, species transport, turbulence and combustion equations. The following sections will describe these equations. [2]

3.4.1 Continuity equation

This equation describes that what goes in should go out. Mass cannot be destroyed or created without sources or sinks. [2]
This equation reads:
\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \]
Eq. 1

### 3.4.2 Momentum equation
Momentum is a vector quantity that is product of mass by velocity vector. In a closed system, momentum cannot be created nor destroyed. It should be conserved. The equation reads: [2]

\[ \partial_j \sigma_{ij} + F_i = 0 \]
Eq. 2

### 3.4.3 Energy equation
Energy equation describes that in a closed system, energy cannot be created nor destroyed. This equation is solved during the simulation to compute temperature field. We chose total energy for this equation which will be discussed in solver section. [2]

### 3.4.4 Species equation
Species equation, like the previous equations, describes that species in a closed systems, cannot be created or destroyed.

This equation reads as follows:
\[ \frac{\partial c}{\partial t} + \mathbf{u} \nabla c = D \nabla^2 c \]
Eq. 3

### 3.5 Turbulence models

#### 3.5.1 k-\(\varepsilon\) Turbulence model
In the following section, turbulence and combustion models are discussed more in details, due to their importance.

The k-\(\varepsilon\) model is one of the most common turbulence models. It is a two equation model which means that two extra transport equations is included to represent the turbulent properties of the flow. This allows the two equation model to account for history effects like convection and diffusion of turbulent energy.

The equation for turbulent kinetic energy is
\[ \frac{\partial (\rho k)}{\partial t} + \text{div}(\rho k \mathbf{u}) = \text{div}(-\rho \mathbf{u}^2 \overline{s}_{ij} - 0.5 \rho \mathbf{u}_i \mathbf{u}_j \mathbf{u}_j - 2 \mu \overline{s}_{ij} S_{ij} - \rho \mathbf{u}_i \mathbf{u}_j S_{ij}) - \frac{2}{3} \rho \overline{s}_{ij} \overline{s}_{ij} \]
Eq. 4

The different terms stands for:

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<tr>
<td>VII)</td>
<td>Rate of production of k</td>
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This formula cannot be implemented in this format, thus it has been change accordingly so it can be implemented.

\[ \frac{\partial(pk)}{\partial t} + \text{div}(pkU) = \text{div} \left[ \frac{\mu_k}{\sigma_k} \text{grad} k \right] + 2\mu S_{ij} S_{ij} - \rho \varepsilon \tag{Eq. 5} \]

and \(\varepsilon\) equation as

\[ \frac{\partial(\rho \varepsilon)}{\partial t} + \text{div}(\rho \varepsilon U) = \text{div} \left[ \frac{\mu_\varepsilon}{\sigma_\varepsilon} \text{grad} \varepsilon \right] + C_{1\varepsilon} \frac{\varepsilon}{k} 2\mu S_{ij} S_{ij} - C_{2\varepsilon} \rho \frac{\varepsilon^2}{k} \tag{Eq. 6} \]

The different terms stands for:

I) Rate of change of \(k\) or \(\varepsilon\)
II) Transport of \(k\) or \(\varepsilon\) by convection
III) Transport of \(k\) or \(\varepsilon\) by diffusion
IV) Rate of production of \(k\) or \(\varepsilon\)
V) Rate of destruction of \(k\) or \(\varepsilon\)

These two equations are solved together in order to solve for turbulence. The \(k-\varepsilon\) model gives good prediction in the free stream and it is less sensitive to values chosen for free stream turbulence properties, it means that this model can model free stream flow to a sufficient degree. On the other hand this model lacks accuracy near wall regions as well as inlets. In Those regions other models should be used like \(k-\omega\). [2]

### 3.5.1 Variations of \(k-\varepsilon\) model

There are variations for \(k-\varepsilon\) model. \(k-\varepsilon\) EARSM is one of the variations which is developed specially for low Reynolds number, thus it can model buoyancy effects very well.

Another variation for \(k-\varepsilon\) model is \(k-\varepsilon\) RNG. This model developed in 1992 to renormalize the Navier-Stokes equations in order to capture smaller scale motions in the fluid. In this method effects of small scale turbulence represented by means of random forcing function in Navier-Stokes equation. [2]

### 3.5.2 \(k-\omega\) SST Turbulence model

In two dimensional thin shear layers, flow changes its directions slowly so turbulence can adapt itself to new local conditions, but in the flows where difference between production and destruction of turbulence is greatly affected by diffusive and convective terms, a compact algebraic prescription for mixing length is no longer a good method. An example of these flows is recirculation flows.

The \(k-\omega\) model, contrary to the \(k-\varepsilon\) model, has better prediction near the walls but it is dependent on the free stream values for turbulence.

The \(k-\omega\) SST formulation is more complex due the fact that it needs a switching or blending function to switch to \(k-\varepsilon\) in free stream or \(k-\omega\) in boundary layers.
The kinematic eddy viscosity, $\vartheta_T$, is defined accordingly:

$$\vartheta_T = \frac{\alpha_1 k}{\text{Max}(\alpha_1 \omega, SF_2)}$$  \hspace{1cm} \text{Eq. 7}

and the k equation reads:

$$\frac{\partial k}{\partial t} + U_j \frac{\partial \omega}{\partial x_j} = P_k - \beta^* k \omega + \frac{\partial}{\partial x_j} \left[ (\vartheta + \sigma_k \vartheta_T) \frac{\partial k}{\partial x_j} \right]$$  \hspace{1cm} \text{Eq. 8}

and $\omega$ equation reads:

$$\frac{\partial \omega}{\partial t} + U_j \frac{\partial \omega}{\partial x_j} = \alpha S^2 - \beta \omega^2 + \frac{\partial}{\partial x_j} \left[ \vartheta + \sigma_\omega \vartheta_T \right] \frac{\partial \omega}{\partial x_j} + 2(1 - F_1) \sigma_\omega \frac{1}{\omega} \frac{\partial k}{\partial x_i} \frac{\partial \omega}{\partial x_i}$$  \hspace{1cm} \text{Eq. 9}

The following expressions are used switch between k-\omega and k-\varepsilon:

$$F_2 = \tanh \left[ \max \left( \frac{2\sqrt{k}}{\beta^* \omega y', \frac{500\vartheta}{y^2 \omega}} \right)^2 \right]$$  \hspace{1cm} \text{Eq. 10}

$$P_k = \min \left( \tau_{ij} \frac{\partial U_i}{\partial x_j}, 10\beta^* k \omega \right)$$  \hspace{1cm} \text{Eq. 11}

$$F_1 = \tanh \left( \min \left[ \max \left( \frac{2\sqrt{k}}{\beta^* \omega y', \frac{500\vartheta}{y^2 \omega}}, \frac{4\sigma_\omega k}{C D_{k\omega} y^2} \right)^2 \right] \right)$$  \hspace{1cm} \text{Eq. 12}

$$C D_{k\omega} = \max \left( 2\rho \sigma_\omega \frac{1}{\omega} \frac{\partial k}{\partial x_i} \frac{\partial \omega}{\partial x_i}, 10^{-10} \right)$$  \hspace{1cm} \text{Eq. 13}

$$\varnothing = \varnothing_1 F_1 + \varnothing_2 (1 - F_1)$$  \hspace{1cm} \text{Eq. 14}

And constants are:

\[\alpha_1 = 59, \quad \alpha_2 = 0.44, \quad \beta_1 = 340, \quad \beta_2 = 0.0828, \quad \beta^* = 0.09, \quad \sigma_{k1} = 0.85, \quad \sigma_{k2} = 1\]

\[\sigma_{\omega1} = 0.5, \quad \sigma_{\omega2} = 0.856[2, 3]\]

### 3.6 Combustion models

Modelling the combustion is one of the most challenging problems in the field of computational fluid dynamics (CFD). In general, complete kinematics of combustion is still unknown. The reason for this fact is the behaviour of combustion itself. Considering that a normal fuel can gives variety of products due the fuel air ratio, pressure, temperature and many other factors, this will results in complex kinematics of combustion. Westbrook and Dryer proposed a model for combustion of fuels based on the facts that:
1- General detailed mechanism cannot be currently included in the most multidimensional problems because of computer size, speed and cost requirements.

2- Detailed mechanisms have been developed and validated for simplest fuel and are not available for most practical fuels.

3- There are many occasions where the great amount of chemical information is unnecessary and a simple two step model would be sufficient.

Westbrook and Dryer have developed two global reaction mechanisms, one-step and two-step. [4,5]

3.6.1 Westbrook-Dryer one–step model

Due the simpler model, this model is faster comparing to two step models. This model can be used where the combustion effects are small and fast results are needed. This model also gives a good estimation of indicator of the expected temperature levels. However, this model got several disadvantages. This model will overestimate $T_{ad}$, adiabatic temperature of flame. This overestimation will grow with increasing the equivalence ratio, which is directly related to increased amount of CO and H$_2$ in the reaction products. Single step model also neglect the fact that hydro carbons are burn in a somewhat sequential manner. This means that CO and H$_2$ are not consumed unless all the hydro carbon fuel is used.

The general formulation of this global reaction mechanism is: [6]

\[
\text{Fuel} + O_2 \rightarrow CO_2 + H_2O \quad \text{Eq.15}
\]

3.6.2 Westbrook-Dryer two-step model

This model is based on two reactions. This results in one big advantage, the ability to treat arbitrary fuels. This is valuable property which makes this model important; however this model has disadvantages too. Two-step model is developed for shock tube ignition delays which make this model not suitable to model flame speed or reaction rate in plug flow or stirred reactors. This model also lacks accuracy to model radical species, thus it does not have enough precision to model NOx formation.

Westbrook-Dryer model two-step model has been chosen since in this project NOx formation is neglected and also the flow is not stirred flow.

The formulation for Methane in this model is as follows:

- Reaction I: \( CH_4 + O_2 \rightarrow CO + H_2O \) \quad \text{Eq.16}
- Reaction II: \( CO + 0.5O_2 \rightarrow CO_2 \) \quad \text{Eq.17}

As one sees, this is a general formulation which can model almost all kind of hydrocarbon fuels. Westbrook and Dryer said that this model will also work for non-hydrocarbon fuels but they didn’t test it.

3.7 Combustion-Turbulence interaction models

Two models are used in this project: Eddy Dissipation Model (EDM), Finite Rate and Eddy Dissipation (FRED). These models are used to solve the interaction between turbulence and combustion.
3.7.1 Eddy Dissipation Model

The eddy dissipation combustion model (EDM) which derives from the eddy dissipation concept is extended to simulate combustion within large eddy simulations (LES). The reaction chemistry is a simple infinitely fast one step global irreversible reaction. The model for the reaction rate is developed from a combination of local kinetics modelling using an Arrhenius law and a new form of the EDC model adapted for LES. The modelling can in principle be applied to both premixed and non-premixed flame and can easily be extended for more complex chemistry. [8]

3.7.2 Finite Rate and Eddy Dissipation

Reaction rates are assumed to be controlled by the turbulence, so expensive Arrhenius chemical kinetic calculations can be avoided. The model is computationally cheap but for realistic results, only one or two step combustion model should be used. [6]

3.8 Flow solution

ANSYS CFX v12.1 was used as solver. The numerical settings for the solver are described below.

3.8.1 Time stepping

The problem is solved as a steady state flow problem, consistent with the RANS turbulence modelling used, which means that relatively large time steps are used in order to achieve a converged solution as quickly as possible. In spite of the turbulence model the flame itself is slightly unsteady, but the oscillations are negligible.

3.8.2 Heat transfer

“Total energy including viscous work terms” model is used, which means that the total energy models the transport of enthalpy including the kinetic energy effects. This model should be used where there is change in density or the Mach number exceeds 0.2; in both of these cases kinetic energy effects are significant. In ANSYS CFX, when one chooses total energy the fluid is modelled as compressible, regardless of the original fluid condition, i.e. gases with Mach number less than 0.2. One should know that incompressible fluid does not exists in reality but for the gases with Mach number less than 0.2 the compressible effects are in general negligible. [6]

3.8.3 Turbulence

For the turbulence both the k-ω SST and the k-ε turbulence models are used. The k-ε model is one of the most common turbulence models. It is a two equation model that includes two extra transport equations to represent the turbulent properties of the flow. This allows the model to account for history effects like convection and diffusion of turbulent energy.

The k-ε model has a good prediction in the free stream, but near the walls, the prediction is poor since adverse pressure gradient is presented. This is not the case for the k-ω which has a good accuracy close to the walls. Based on this idea Menter (1992a) invent a model that called SST k-ω which uses a transformation of k-ε in to k-ω near walls and k-ε model in the fully turbulent regions far from walls.

For wall treatment scalable wall function is used. Standard wall functions are based on the assumption that the first grid point off the wall (or the first integration point) is located in the universal law-of-the-wall or logarithmic region. This helps to have
higher aspect ratios which means reduce density of mesh near the walls. This results in lower computational costs but it will also reduce the accuracy because high aspect ratio results in high round off errors. On the other hand, standard wall function formulations are difficult to handle, because it should have high resolution near walls means higher computational costs. Also if the resolution becomes too fine, the first grid spacing can be too small to bridge the viscous sub layer. In this case, the logarithmic profile assumptions are no longer satisfied. The user should make sure that both upper and lower limit for the grid size are not crossed. Recently, alternative formulations (scalable wall functions) have become available, Menter and Esch, which allow for a systematic grid refinement when using wall functions. [7]

3.8.4 Combustion model

Westbrook-Dryer two-step model was used for combustion. This model is mainly focused on the modelling of the combustion at temperatures above 1000K. At these temperatures experimental data are usually hard to gather due the small time scales, usually in the order of micro seconds, but on the other hand reactions simpler formulations. This method is mainly used for hydrocarbon fuels at high temperatures, however Westbrook and Dryer state that using the same method, one can develop relations for other non-hydrocarbon fuels. [4]

3.9 Convergence criteria

In order to determine if convergence is obtained, residuals are constantly monitored and when they are reasonable flattened out, after 10,000 iterations, the run is stopped and the results are post-processed.
4 Results and post processing

The grid sensitivity study was performed on four different mesh sizes, 400,000 (400K), 500,000 (500K), 1,000,000 (1M) and 2,000,000 (2M) cells. The aim of this study is to obtain a mesh size were the results are grid-independent. Furthermore, two different turbulence models were used in the study, the k-ε and the k-ω SST model.

The comparisons were done considering the temperature, the pressure, the axial velocity and the major species, CH₄, CO₂ and CO.

These properties are calculated on seven locations: mid plane, YZ, YZ1, YZ2, YZ3, YZ4 and YZ.

Mid plane is the bisector of the burner chamber. The other planes are located in the burner. To address the planes we use a dimensionless number as percent. it means how far they are from the combustion chamber entry, 0% and 100% locations are shown in the Figure A1, in the appendix section. The locations of the plane are as follows:

1- YZ @ 0.000%
2- YZ1 @ 3.846%
3- YZ2 @ 9.587%
4- YZ3 @ 18.197%
5- YZ4 @ 26.808%
6- YZ5 @ 41.159%

4.1 Case one

In this section we discussed the obtained results for different cases

The following cases are for the grid study, which means that all the settings are the, but the number of cells is different. The following settings were used:

4.1.1 Temperature

The left column shows the temperature contours at YZ planes and the right side shows temperature at mid plane. From up to down: 400K, 500K, 1M and 2M cells. This implies that the temperature results are independent of number of cells.

4.1.2 Recirculation zones

Figure 12 shows the recirculation zone inside the domain, which means that the axial velocity is in opposite direction to the flow field. Top row: 400K (left) and 500K (right); Bottom row: 1M (left) and 2M (right). These regions look similar with each other. It implies that the recirculation zones are independent of number of cells. In
each picture two major recirculation regions are illustrated, one is around the vane and other one is in the chamber.

![Figure 14. Reverse velocity](image1)

The left side shows the reversed velocity contours at YZ planes while the right side shows the reversed velocity at mid plane. From up to down: 400K, 500K, 1M and 2M.

### 4.1.3 CH$_4$ Mass fraction

![Figure 15. CH$_4$ Mass fraction](image2)

Figure 15 shows CH$_4$ mass fraction contours at YZ planes at the left side. The right side shows CH$_4$ mass fraction at mid plane. From up to down: 400K, 500K, 1M and 2M.

CH$_4$ mass fraction is a good parameter to see exactly where the burning occurs or in case of unburned gases, how much leakage exists via outlet.
4.1.4 CO Mass fraction

Left side shows CO mass fraction contours at YZ planes while the right side shows CO mass fraction at mid plane. From up to down: 400K, 500K, 1M and 2M. CO mass fraction can show us the shape of flame since, in ideal case, CO only exists within flame. Also in these Figures one can trace leakage of CO to environment which is a safety parameter.

4.1.5 Profile study

In this section we will study area average values of properties on YZ1, YZ2, YZ3 and YZ 5. Note that span is 0 at centre line and 1 at walls and it varies linearly, it is dimensional less coordinates.

Figure 17. Pressure profile at different YZ planes

Figure 17 shows pressure distributions along the YZ planes. In the converged solution, fluctuations exist and small variation in pressure profile is due this fact.
Temperature profiles are also possessing fluctuations, due the convergence as mentioned before, but these fluctuations are highest near tip of flame area (YZ 2 and YZ 3). While near outlet (YZ 5) and inside the flame area (YZ 1) these fluctuations are less.

As the flow approaches to the farther planes, concentration of CH$_4$ will decrease, as they used up in the reactions.

CO$_2$ will increase as flow moves toward the exhaust, because CO$_2$ is the product of combustion.
Despite the fact that those profiles are not exact match but they have good manner, one can decide and use 500,000 meshes case for the rest of solution without concerns of grid study or inaccurate answer.
4.1.6 Tables

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Figure 23. Data table for case 1, from top to bottom: 400K, 500K, 1 M and 2 M

These are numerical values for parameter average on the YZ planes. These values can use to compare results more accurately.

4.1.7 Result discussion

Aim of these set of tests is to do grid study. 2M cells case shows a strange behaviour in some tests, which cannot be avoided by re doing the tests, but the other three cases’ results are similar with each other. This means that the grid study is so far good and all the cases can be used. We choose further on 500K case, which is cost efficient and also not the lowest mesh density. There exists a circulation zone in front of ignition inlet; this region is one of the most important regions in order to mix flow and better flame.

The combustion –turbulence interaction model that used was eddy dissipation, this can results in unrealistic combustion model. In further test two other methods will be used, finite rate and eddy dissipation (FRED).
4.2 Case two

This case is also a grid study which means we are going to study four different meshes, but all have same solution setting.

Settings are:

Turbulence model: k-ω SST, Wall function: Automatic, Heat transfer: Total energy with viscous work term, combustion model: Finite Rate and Eddy Dissipation

Boundary conditions are same except for the ramp part of the wall, which is set to free slip in order to avoid strange numerical error and flashbacks.

4.2.1 Temperature

![Temperature contours](image.png)

*Figure 24. Temperature contours*

Left column shows temperature contours at YZ planes while the right column shows temperature at mid plane. From up to down: 400K, 500K, 1M and 2M

Despite the fact that these graphs are different with previous case, but they all still have the same pattern. As one can see flame tip is more stretched than the previous case.
4.2.2 Recirculation zones

Figure 25. Recirculation zones; Top row: 400K (left) and 500K (right); Bottom row: 1M (left) and 2M (right)

Figure 26. Reverse velocity

Left column shows reverse velocity contours at YZ planes while the right column shows reverse velocity at mid plane. From up to down: 400K, 500K, 1M and 2M. These two Figures show the separation zones. There are circulations in red areas in the Figure 26 which will mix fuel with air more.
4.2.3 **CH₄ Mass fraction**

![CH₄ Mass fraction contours](image)

*Figure 27. CH₄ mass fraction contours;*

Left column shows t CH₄ mass fraction contours at YZ planes while the right column shows CH₄ mass fraction contours at mid plane. From up to down: 400K, 500K, 1M and 2M. This case, compared to case 1, has early flame. This means that there is less CH₄ Mass fraction exists downstream in combustion chamber. Yet same as previous case there is no trace if CH₄ far downstream, meaning that this burner has a safe burning for environment.

4.2.4 **CO Mass fraction**

![CO Mass fraction contours](image)

*Figure 28. CO mass fraction contours;*

Left column shows CO mass fraction contours at YZ planes while the right column shows CO mass fraction contours at mid plane. From up to down:400K, 500K,1M,2M
Flame shape can be predicted by looking at CO mass fraction. One can see that the pattern for 2M case is bit different with other cases. That can be due the numerical fluctuation in answer or numerical error.

4.2.5 Profile study

In this section we will study area average values of properties on YZ1, YZ2, YZ3 and YZ 5.

![Pressure profile at different YZ planes](image1)

*Figure 29. Pressure profile at different YZ planes*

These profiles shows that all cases have same pressure distribution, however at profile of YZ2 one can observe a jump, which present a numerical error in solution for that point rather than a important physical fact.

![Temperature profile at different YZ planes](image2)

*Figure 30. Temperature profile at different YZ planes*

Temperature profile plotted in these pictures. All the cases follow the same behaviour except for the 2M case, it seems that we have a problem in setting up this case but since all the other three cases agrees with each other; again it seems that this odd behaviour is due to the numerical error rather than a physical fact.
Figure 31. CH₄ Mole fraction profile at different YZ planes

Figure 32. CO₂ Mole fraction profile at different YZ planes

Figure 33. CO Mole fraction profile at different YZ planes
From Figures 29 to 34, one may observe strange behaviour of the 2M case. The pattern of 2M case does not follow the other cases; however error is small and can be neglected. If one interested in acquiring better results he or she needs to either re mesh or re run it. Due the limitation in time, this cannot afford in this project. Yet we meet our goal, other three cases have the same behaviour and thus 500,000 can be accepted.

4.2.6 Tables

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Figure 34. Axial velocity profile at different YZ planes

Each value is area averaged for that quantity on the represented plane. i.e. T(ave) on YZ 1 is average temperature for that plane. This is one of the best tools to compare the results of different cases.

4.2.6.1 Results and discussions

In the case 2M, exist differences with the other cases. It can be due different reasons i.e. bad quality of meshing or numerical errors in solver. However this error is not
critical since it is a case study and it seems that the 500K case agrees with the results we expected.
5 Turbulence and heat transfer model study

In the previous two major cases, we have done grid study on a generic gas turbine combustor. From the results, we choose 500,000 cells case, which presents both accuracy and numerical speed.

In the following case we will use other variations in the turbulence models. Heat transfer is also including for some of the cases in the study.

General boundary conditions and working condition are mentioned in section 3.3, but for each of following cases, just one of settings was changed. New cases are:

- Case a: Turbulence model k-\(\varepsilon\) EARSM
- Case b: Turbulence model k-\(\varepsilon\) RNG
- Case c: Including conduction and convection with ambient using thin wall interface, free stream temperature of 600K
- Case d: Turbulence model: k-\(\omega\) SST, combustion model: finite rate and eddy dissipation
- Case e: Top wall has heat transfer coefficient of \(54.459 \frac{\text{w}}{\text{m}^2\text{k}}\)

Used heat transfer coefficient was calculated. Calculations are shown in the appendix, section 7.2.

5.1 Software limitation for thin wall interface

In order to model conduction and convection, we use thin wall interface, a new feature in ANSYS CFX 12.1. The limitation of software implies that this interface should be within the computational domain but not as a boundary. Thus we have to add an additional domain to previously meshed domain which is illustrated in Figure 36. All the boundaries of this additional domain are opening with atmospheric pressure.

![Figure 36. Additional domain](image)

5.2 Case three

In this case different features of different models will be discussed. As mentioned in section 5, different models will be used. Aim of this case is to compare results based on different turbulence models or heat transfer models.
5.2.1 Temperature

![Temperature Contours](image1)

*Figure 37 Temperature Contours;*

Temperature contours are illustrated for different cases. As one can see the patterns are not same especially for Case c; where heat transfer enabled via interface. Temperature distribution for Cases c and e is affected by cooling from fresh air above. In the Figure 37 from top to bottom: Case a, Case b, Case c, Case d and Case e.

5.2.2 Recirculation zones

![Recirculation zones](image2)

*Figure 38 Recirculation zones*

Recirculation zones are illustrated in the Figure 38. These zones are affected by both turbulence model and heat transfer model.
Reverse velocity contours are illustrated in the Figure 39. Together with Figure 38, these Figures show the recirculation zones. Circulation regions around the vane should be minimized in the design because they represent losses in those regions. In Figure 39 from top to bottom: Case a, Case b, Case c, Case d and Case e.

5.2.3 CH₄ Mass fraction

CH₄ mass fraction contours are shown in the Figure 40. Case c, Case d and Case e show different patterns. Flames are extended in these cases. In Case c and e, where heat transfer exists, due to the reduction of temperature, some portion of injected fuel cannot be burned at the start of combustion chamber. But as the unburned fuels goes down in the combustion chamber, it will warm up and burns. Case d here shows strange behaviour. This can be errors in calculating flow field in the chamber. Also ANSYS will calculate and adapt mesh automatically near the walls, thus this error can be made because of bad mesh adaption. In the Figure 40 from top to bottom: Case a, Case b, Case c, Case d and Case e.
5.2.4 CO Mass fraction

Figure 41 CO mass fraction contours

Figure 41 shows the contour plot of CO mass fraction at different plates. This can be a good measure to plot the flame. We assume that all the fuel will be burned, thus where the CO exists, as written in Eq.17, there is still one step of reaction remains. In the other word reactions exist in the areas with trace of CO. These Figures are instantaneous pictures of the events happen inside the combustion chamber. The shape of flame in these plots will change depend on when the iterations has been stopped, that is the reason average values and plots will be used to compare the results.

5.2.5 Profile study

In this section, data presented as a curve versus span. Span range is from 0 to 1. 0 means the point is in the centre line while 1 represents points on the outer walls. Data presented in the chart are annular average. It should be mentioned that for the case c, span includes additional domain.
As it is shown in the Figure 42, it seems that case a and case b agree with each other while case c, d and e agree with each other. The reason behind this fact is due the turbulence models. Two first cases use variations of k-\( \varepsilon \) while the three later cases use k-\( \omega \) model. Based on the theory section, section 3.5, k-\( \omega \) model should present a better estimation of boundary layer, thus more accurate calculations of pressure.

![Figure 43. Temperature profile](image)

One can expect that case c and case e would have lower temperature due the heat transfer, and this illustrated in the Figure 43. In the cases c and e, at the beginning of the chamfer, YZ 1 in Figure 43, flow temperature is highly affected by the ambient temperature, as one can see only 40% of span reaches the final temperature of 2000K. As the flow moves forward it will be heated. In YZ 5 in the Figure 43, approximately 90% span reaches the final temperature, or after flow moves 41% of its path. On the other hand, for the cases without heat transfer, after flow moves to YZ 2 or 10% of its path, the flow reaches its final temperature.

![Figure 44. CH\(_4\) mole fraction profile](image)
In Figure 44, fuel consumption can be traced. As one can see, on early stages, YZ 1, there is fuel. Fuel will be burned as the flow moves down its path. By comparing Figure 44 with Figure 43, one can see that when most parts of span reaches the final temperature, there is no fuel left. For the cases without heat transfer, fuel will be consumed when it reaches 10% of combustor length while in the case c, fuel will still be presented even in the middle parts of combustors. In Figure 44, case d shows a strange behaviour, as mentioned in section 5.2.3, it can be due the numerical errors.

![Figure 45. CO mole fraction profile](image1)

CO mole fraction profiles are illustrated in the Figure 45. As mentioned in section 3.6, CO exists on the zones with flame, since it is a middle production and will be consumed on the later reactions. As Figure 45 suggests, as the flow goes down the stream, fuel will be consumed thus there is no source to produce CO. But one should notice that based on Figure 41 and section 5.2.4, CO profiles are sensitive to iterations because in the reality shape of flame will change.

![Figure 46. CO₂ mole fraction profile](image2)

CO₂ is the one of the final products. One expects that as flows move down stream, mole fraction of CO₂ increases, and that can be seen from Figure 46. However in the
case c and case e, production rate of CO$_2$ is less than other cases. As mentioned before the reason behind this fact is due the cooling effects of environment, reaction rate of combustion will drop, thus less CO$_2$ will be produced compared with the cases without heat transfer.

Figure 47 shows the velocity profiles. General direction of the flow is in the negative direction thus at the span ranges that velocity profile is positive, recirculation zones exist or in the other words, those are the regions with the reversed flow velocity.
### 5.2.6 Table

<table>
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<th>CH₄</th>
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<th>CO</th>
<th>CO₂</th>
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In this Figure, average values for different parameters are calculated. As one can see highest average amount of CH₄ in these cases belongs to case c, where heat transfer exists. T_max is almost same among the mid plane, YZ 3, YZ 4 and YZ 5. In YZ 1 and YZ 2, T_max differ for each case due the different pattern for flame shape.

### 5.3 Results and Discussion

In the section 4.1 and 4.2 different turbulence models tested. Each model was tested on four different grids, and it was shown that the results for each model are grid independent, however these models simulate the flow field in a different manner. One can expect that 500,000 cells case would be sufficient number of cells to work for the next case. In the section 5.2 the grid structures are same for all the cases and it was 500,000 cells, but different settings were used and the results are compared with each other. As expected, different models offer different flow field models. By enabling the heat transfer pattern of flame will change. Heat transfer plays an important role in the functionality of the burner. As it is illustrated in the cases c, d and e, if the flame reaches the outlet of device, it could result in damaging the turbines blade and also unburned carbohydrates. Best model can be chosen only after validation with experiment.
6 Conclusion

It should be mentioned in the pressure plots and pressure profile of cases, pressure distribution may vary with number of iteration and that is the reason the plots and charts may vary. The variation of the pressure fall into acceptable error range for numerical error, thus the results were accepted.

The conclusion from the grid-study is that the mesh-size that is used for the 500K case is enough, or in other words the results are grid-independent. These conclusions are based on steady-state simulations and were not tested on transient simulations due to limitations of time in the project. This is also important to check in the future work. The 500k mesh size would imply that the number of cells for a full 360\degree model would be approximately 16M cells.

By consider all the three cases; the recommendation is to use the k-\(\omega\) SST model with heat transfer for the steady-state simulations. Because this model showed stable convergence and also it predicts flow field better than the other cases.

6.1 Future works

The suggestion for future work is to test more models. Also, the simulations done in this work uses CH\(_4\) as fuel, while there are varieties of fuels available to use.

Suggestion for future work:

- Test the open source software OpenFOAM
- Test different fuels
- Modelling the generic gas turbine combustor with different inlets for fuel and air and use pre heated air.
- Grid study for transient simulations
7 References

6- ANSYS CFX® v12.1 User Manual
7- J.C. Kok, Resolving the dependence on free stream values for k-omega turbulence model, Nationaal Lucht- en Ruimtevaartlaboratorium, 1999
8- R. J. A. Howarda, D. Toporovb, The eddy dissipation combustion model developed for large eddy simulation.

7.1 Picture references

p2- http://www.bloodhoundssc.com/car/jet_propulsion.cfm
p3- http://www.citizendia.org/Turboshaft
8 Appendix

8.1 Pictures

Figure A1, YZ planes

Figure A2, Ideal Brayton cycle

8.2 Heat transfer coefficient calculation

In order to calculate heat transfer coefficient, a test case has been carried out. As it shown in the Figure A3, test case consists of a steel plane of thickness of 2mm in the middle, and two entrances for air. Cold air enters at 600K while the hot cold enters at 1800K. Heat transfer coefficient calculated using the build in calculator in the CFX-Post. Both cool air and hot air enter with velocity of 20 m/s.

Figure A3, Test case for calculating h