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CFD Analysis of the Combustion Process Evolved in the TKT-1 Academic Jet Engine

Combustion is a complicated process induced by a chemical reaction in which fuel combines with the oxidiser, usually oxygen already in the air to generate heat. Investigating combustion is important for increasing energy efficiency and a key component for further greener solutions and cleaner developments. With the help of CFD modelling, clearer visualisation and a better comprehension of thermal properties can be revealed. Understanding those specific thermal properties will allow the accurate and efficient comparison between different types of fuels. Hence, this paper aims to model the combustion in a TKT-1 research turbine engine using fossil standard fuels and collect the combustion emissions parameters to be able to conduct a correct comparison to the same process when sustainable fuels (SAFs) are used.

Keywords: *CFD analysis, combustion simulation, combustion chamber outlet gas emissions, TKT-1 combustion chamber modelling, fossil fuel, sustainable fuel*

1. Introduction

The constant progress and development in the aviation sector have shaped this industry's futuristic needs and goals. Since all eyes are focused on greener and more environmental-friendly solutions, one cannot neglect the effect of aviation propulsion systems' emissions, especially in the case of jet fuel engines. According to recent studies, the emissions exhausted from the jet engine contain large amounts of nano-sized particles, which are capable of reaching the lower airways upon inhalation [1].

This increasing need to lower the negative effects of such engines has opened the door for countless studies and investigations in the field of sustainability. The real focus was on delivering the best of jet engines efficiency-wise while reducing greenhouse effects as much as possible. While the final aim of the scientific world is to reach a 100% clean energy source for fueling jet engines, one can easily say that it is still relatively far away from that aim, and it will be unreasonable and uneconomical to scrap and/or modify all already manufactured aircraft and engine configurations to achieve that particular end goal. Hence, new research has emerged to accommodate the old configurations and decrease the negative impact of jet fuel engines by introducing Sustainable Aviation Fuels (SAF). The key point is to mix an adequate amount of SAF fuels with Jet-A fuels to reduce emissions but at the same time keep high thrust reliability and availability.

However, knowing the optimal mixing proportions between the Jet-A and the SAF fuels is only possible if the thermal properties of the combustion process and the turbine gas inlet emissions are accurately measured and collected for the sake of proper academic comparison. Therefore, in this paper, those properties will be collected by using Computational Fluid Dynamics (CFD) tools to perform virtual tests on a TKT-1 academic turbojet engine combustion chamber operation in a precise way. Despite the widespread use of CFD in gas turbine simulations, academic turbojets like the TKT-1 provide unique challenges due to their small size and fast rotating speeds, necessitating careful model selection and validation. Previous research on bigger gas turbines has laid the groundwork for combustion and emission modelling, but few have addressed the unique characteristics of small-scale engines. The current study seeks to address this gap by using CFD techniques to investigate the combustion process and gas emissions in the TKT-1 engine under a variety of operational situations to give insights into enhancing the performance and environmental effect of academic turbojets by analysing the exhaust parameters.

2. Combustion process

Combustion is a complicated chemical reaction in which a fuel combines with the oxidiser, usually oxygen existing in the air, to generate heat. Understanding combustion is important for increasing energy efficiency and lowering environmental impact.

The general chemical formula for a hydrocarbon combustion process [2]:

$$C_xH_y + \left(x + \frac{y}{4}\right) O_2 \rightarrow xCO_2 + \frac{y}{2} H_2O + Heat \nearrow \tag{1}$$

Some previous researchers have been able to model the combustion process of different jet fuels to predict the emission performance of the fuels. However, due to the high complexity of the composition of the jet fuels, many authors have chosen a more simplified approach. Jet fuel is modelled by using what is known as surrogate fuel, which has a more simplified composition in comparison to the real fuel, i.e. fewer components. The advantage of surrogate fuels is that the combustion characteristics of the real fuel can be modelled in a satisfying way using a simplified mixture of fuels [3], in our CFD simulation to reduce the complexity of the complicated mixture of hydrocarbons, kerosene (Jet A) has been defined in the CFX-RIF tool with only two components [4], [5], [6]:

- 60% $C_{10}H_{22}$ (n-alkanes, iso-alkanes)
- 40% C_9H_{12} (aromatic)

Based on Equation (1), the total amount of the required O_2 for kerosene is:

$$kerosene + 14.1\ O_2 \rightarrow 9.6CO_2 + 9H_2O + Heat \nearrow \tag{2}$$

According to the CFX-RIF tool, the default O_2 percentage is 23.3% in the air. We can calculate the optimum theoretical fuel/air ratio based on the previous formula.

2.1. Flame types

To select the best combustion model in CFX, it is important to understand the flame types which can be classified into three main categories [7] based on the pure fuel and pure oxidiser entering the combustion zone as illustrated in Figure 1. The characteristics of each flame type are highlighted in Table 1. The first characteristic is the non-premixed flames, the fuel and oxidiser (usually air) are not mixed before they reach the combustion zone, they diffuse together at the combustion zone where the flame forms. The second one is the premixed flames, the fuel and oxidiser are mixed before they reach the combustion zone. And finally, the third is the partially premixed flames, which are intermediate between premixed and non-premixed flames. In these flames, the fuel and oxidiser are mixed partially before they reach the combustion zone, but there is still some degree of mixing occurring at the flame front.

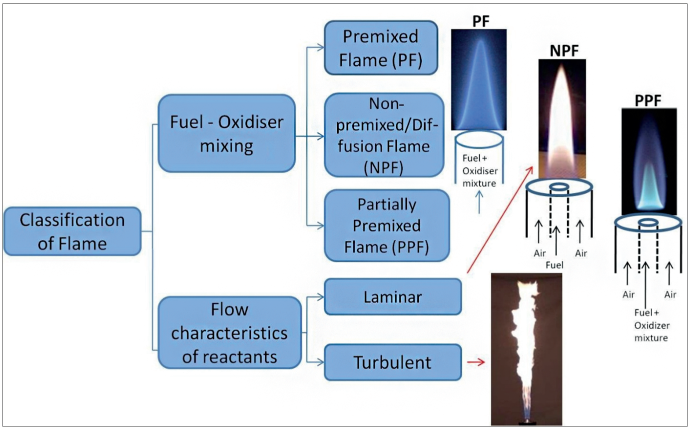


Figure 1.
Classification of flame types [8]

Table 1.
Comparison of flame types [9]

Flame Type	Fuel/Oxidiser Mixing	Characteristics
Premixed	Mixed before combustion	High efficiency, controlled flame, risk of flashback
Non-Premixed	Mixed at the combustion zone	Diffusion-controlled, inhomogeneous, safer from flashback
Partially Premixed	Partially mixed before and at the combustion zone	Balance of control and safety, variable mixture

2.2. Damköhler number (D_a)

The TKT-1 turbojet engine is equipped with a can-annular combustion chamber containing 4 chambers with 4 fuel nozzles. The flame type in this engine is non-premixed flame because fuel and air are not mixed before they enter the combustion zone. Another factor that must be taken into consideration for selecting the best combustion model in CFX is the Damköhler number.

Combustion depends directly on mixing and chemistry. The ratio of the turbulent mixing time to the chemical reaction time is known as Damköhler Number *(D_a)* which is a dimensionless number:

$$D_a = \frac{Mixing\ Time\ Scale}{Chemical\ Time\ Scale} \tag{3}$$

If $D_a \gg 1$, the chemical reaction rates are fast, the reaction progress is limited by turbulent mixing. When the $D_a \ll 1$, the chemical reaction rates are slow, the reaction progress is limited by chemical kinetics. In jet engine cases the $D_a \gg 1$ and so the chemical reaction rates are fast [7].

3. CFX combustion models

ANSYS CFX, a Computational Fluid Dynamics (CFD) software provides many combustion models for simulating various combustion processes. Selecting the correct combustion model is determined by the individual application and the nature of the combustion process under investigation [5], [10].

The main available models in ANSYS CFX based on the combustion mode can be Non-Flame Mode or Flame Mode. Eddy Dissipation Model (EDM), Finite Rate Chemistry (FRC) Model, or the Combined Model (EDM + FRC Model) models can be used for the first mode. But for the second mode, the known combustion models are the Pre-mixed/Partially Premixed: Burning Velocity Model (BVM), the Extended Coherent Flame Model (ECFM), or the Probability Density Function (PDF) Flamelet [10], [11].

As it is mentioned in the previous section, the chemical reaction rate is short, so it plays the main role in the reaction progress ($D_a \gg 1$) in the TKT-1 combustion chamber. It is a non-premixed flame, so the most effective model in this case is the Probability Density Function (PDF) Flamelet. The interaction theory is based on the Phase Field Method (PFM) combustion model and turbulence in the flow field. Combustion is thought to occur in thin sheets known as flamelets. The turbulent flame is shown as a collection of laminar flamelets.

To use the PDF flamelet model first, it is required to create the flamelet library for the investigated fuel from detailed kinetic schemes, the flamelet library will be used while running the solver as illustrated in Figure 2. Generating this flamelet library can be done using the "CFX-RIF" tool which was developed by Prof. Peter's group in Rheinisch-Westfälische Technische Hochschule (RWTH), Aachen [11].

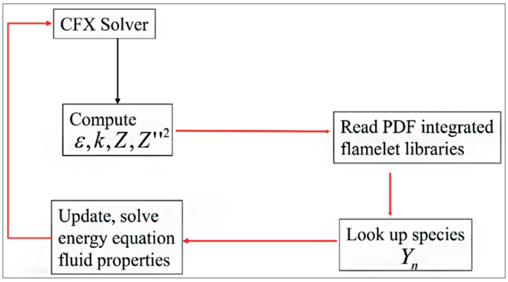


Figure 2.
Implementation of PDF Flamelet library in CFX [11]

NO_x is one of the reactive gases that will form nitrous acid on release into the atmosphere. In other words, it is formulated when the fuel is burned in the air at high temperatures. In addition to the previous reaction models, supplementary models are needed for simulating the combustion process in the combustion chamber of turbojet engines in order to model pollutants (NO_x and Soot). These models are: the Thermal NO – thermal decomposition of N_2, Prompt NO – hydrocarbon radical attack on N_2, the Fuel Nitrogen – release of fuel-bound N compounds, the Reburn NO – the destruction of NO in fuel-rich flames, and finally the N_2O – alternative thermal NO_x mechanism. However, for the sake of this paper, the thermal formation model will be used to simulate the burning of NO_x [12], [13].

4. CFX simulation process

Before starting the simulation process, it is necessary to understand the can-annular type structure of the typical combustion chamber as shown in Figure 3.

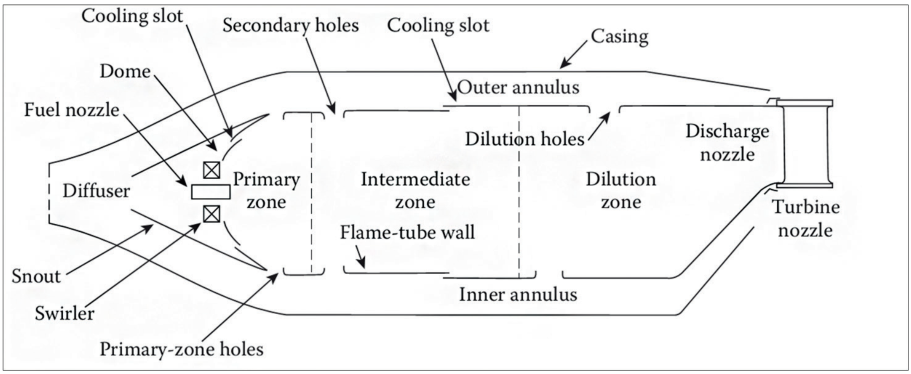


Figure 3.
Structure of the typical combustion chamber [14]

TKT-1 academic jet engine combustion chamber is rather unique. The structure of it is presented in the cross-section in Figure 4.

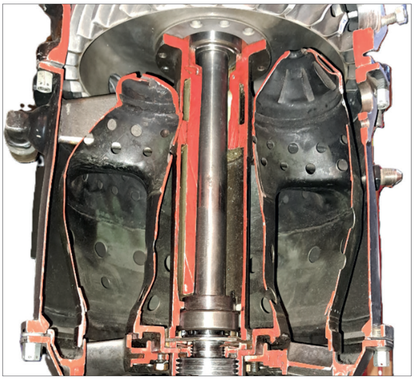


Figure 4.
TKT-1 combustion chamber cross-section [the authors]

To start the simulation process, the geometry needs to be imported and prepared for the modelling process, and then for creating the mesh, only ¼ of the combustion chamber geometry was decided to be considered in this study because the combustion chamber has a symmetrical shape allowing the size reduction of the investigated geometry which leads to the ability to use a higher number of cells while ensuring more accurate simulation and a shorter overall calculation time.

The fuel enters the combustion chamber from a 0.8 mm diameter circular surface, thus the finest mesh is used with a 0.01 mm element size. The global volume is meshed with 4 mm large elements and mesh refinement is applied on the specific walls shown in Figure 5. Inflation layers are used with a 2 mm total thickness and 1.1 growth rate. The inflation layer is built up from 10 layers. Furthermore, due to the importance of the primary and intermediate zones of the combustion chamber, three spheres have been defined in front of the fuel nozzle axis the size of whose elements increases with further distance from the nozzle. The final mesh can be seen in Figure 5 which is built up from 28,638,128 elements and contains 7,744,980 nodes.

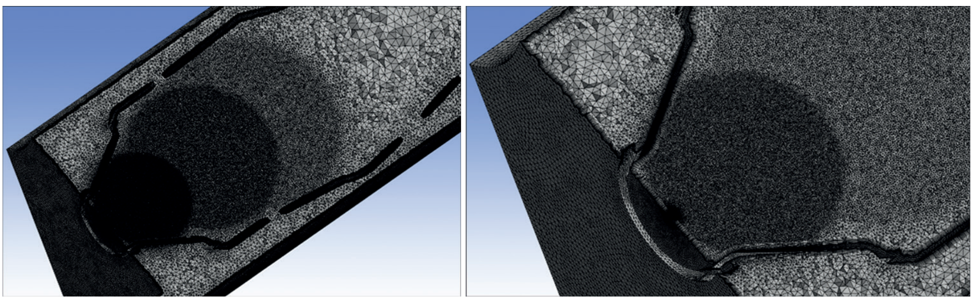


Figure 5.
TKT-1 combustion chamber mesh cells [the authors]

The CFX model needs to simulate the actual combustion process, therefore it was necessary to define the boundary conditions accurately of the built model. Figure 6 shows the conditions used for the boundary conditions and the parameters that form the engine's artificial environment [5], [6]. The set boundary parameters in the below-listed figure are for a full engine thrust level (100%).

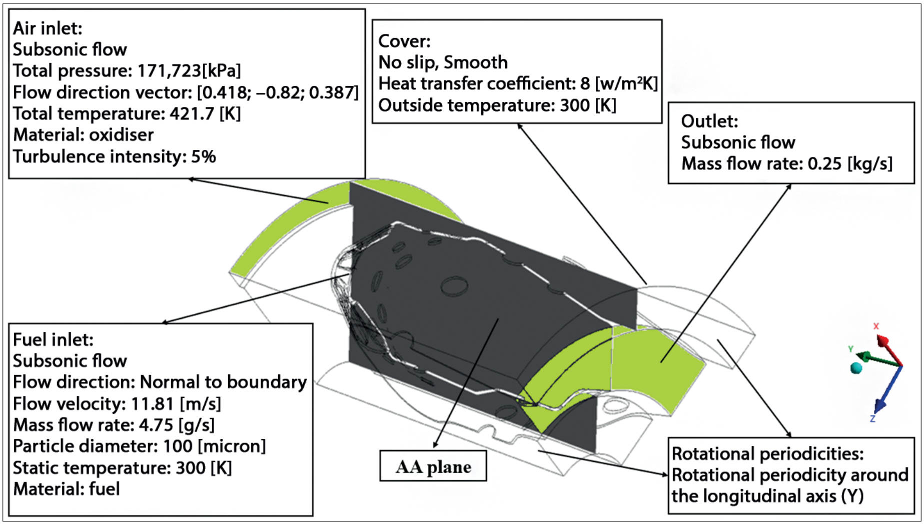


Figure 6.
Boundary conditions for the CFX model [the authors]

The fluid dynamics in the combustion chamber are turbulent and involve heat transfer processes combined with reaction kinetics. The conservation of mass, momentum, and energy equations must be solved numerically in addition to the basic governing equations. In this simulation, the standard k-epsilon turbulence model and the P-1 radiation model are used for further investigation and analysis. Furthermore, a non-premixed combustion model with a PDF mixture fraction approach is applied as stated above, where fuel and oxidiser are introduced separately in the reaction zone [15], [16].

To enhance the simulation accuracy, the High-Resolution advection scheme and the High-Resolution turbulence model discretisation scheme were used. The advection scheme can help minimise the numerical diffusion and ensure precise transport of flow properties such as momentum and energy especially in areas with steep gradients that are subject to shock waves or boundary layer conditions. As for the turbulence model discretisation scheme, it is used because it can predict turbulent behaviour by capturing the complex structure of the flow. Combined together these two schemes can assure the robustness of the solution regardless of the flow conditions [17].

The setting for the liquid phase was the Lagrangian Particle Tracking since it is known for creating an accurate analysis of particle behaviour in a fluid flow. This method tracks individual particles, such as droplets or solid particles, as they move through the flow field, providing insight into their interactions with the fluid, including drag, collisions, and heat or mass transfer. Unlike Eulerian methods, which treat particles as a continuous phase, Lagrangian tracking follows each particle's trajectory, offering a more precise representation of particle dynamics, and since the flow in this research is a multiphase flow where particles and fluid phases interact, Lagrangian Particle Tracking approach excels in precision to other methods [18].

The Primary Breakup Blob Method, Schiller-Naumann Drag Force, and Ranz-Marshall Heat Transfer models are crucial for simulating droplet behaviour in multiphase flows. The Blob Method simplifies the complex breakup of liquid into droplets, while the Schiller-Naumann model accurately calculates the drag force on particles, determining their movement through the fluid. The Ranz-Marshall model estimates heat transfer between droplets and the gas, helping to predict evaporation or temperature changes in processes like fuel injection. Together, these models provide a comprehensive understanding of spray dynamics [10].

5. CFX simulation results

After creating the appropriate mesh and choosing the most adequate settings, the built model was run through the CFX solver to gather the analysis. The residual and imbalance balance values are within an acceptable level (below 2%) shown in Figure 7, which showcases that all obtained parameters for the study case were reached after 150 iterations. Additionally, as illustrated in Figure 8, a monitor point was set for the outlet average temperature which is inside the range of acceptable values after 150 iterations.

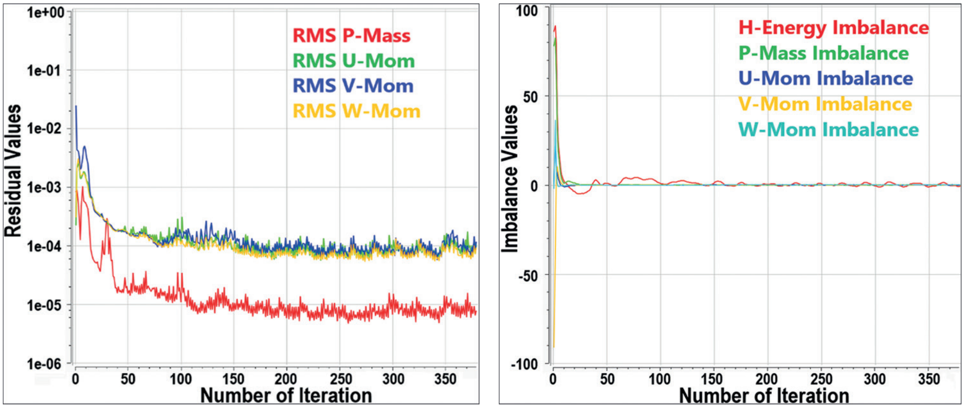


Figure 7.
Residual values (left) and imbalance values (right) [the authors]

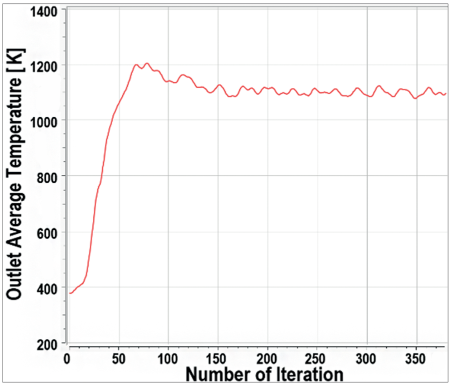


Figure 8.
Outlet average temperature [K] [the authors]

Figure 9 displays the temperature distribution on AA and outlet planes, and the combustion chamber outlet average temperature is 1135.3 [K]. This temperature will be used in future research for comparison reasons with the utilisation of SAF fuels.

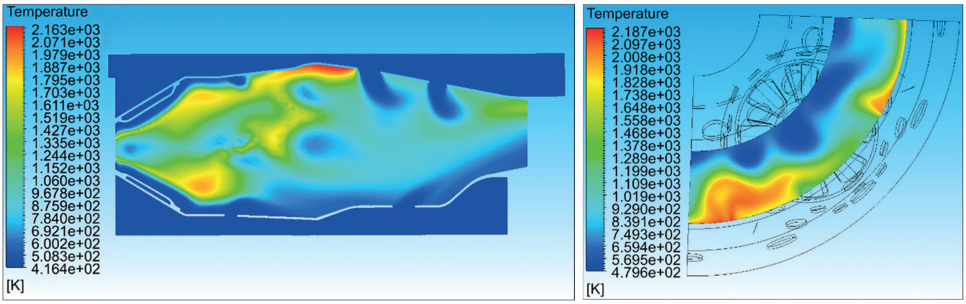


Figure 9.
Temperature distribution: AA plane (left), outlet plane (right) [the authors]

Figure 10 illustrates the total pressure distribution on the AA plane. From these results and based on the function calculator in CFD-POST, the total pressure decreased from the inlet to the discharge nozzle (turbine nozzle) by 5.19%, which can be calculated from the pressure recovery factor equation for the combustion chamber (r_{cc}):

$$r_{cc} = \frac{average\ total\ pressure\ at\ outlet}{average\ total\ pressure\ at\ inlet} = \frac{257.32\ [kPa]}{271.42\ [kPa]} = 0.948 \qquad (4)$$

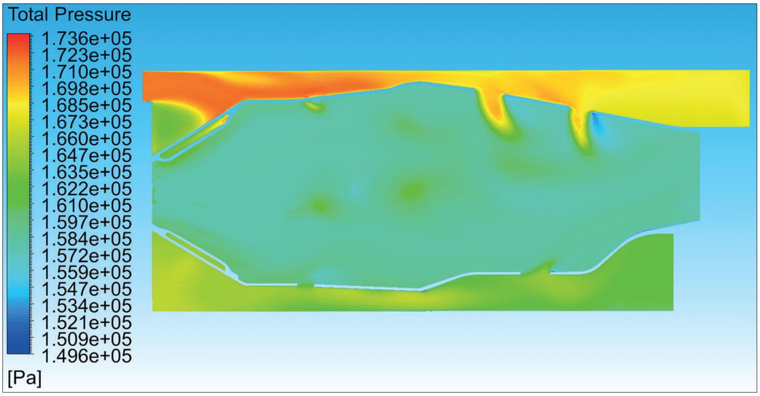
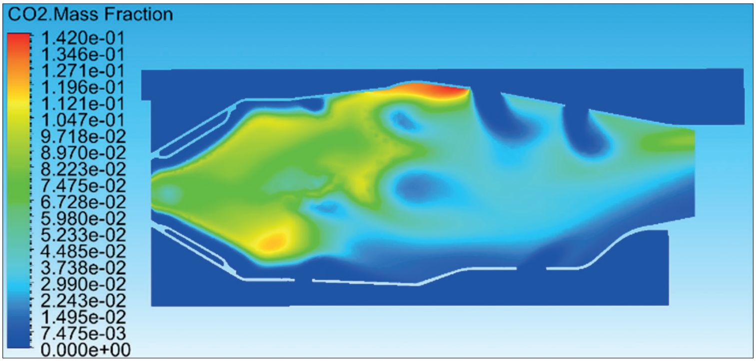
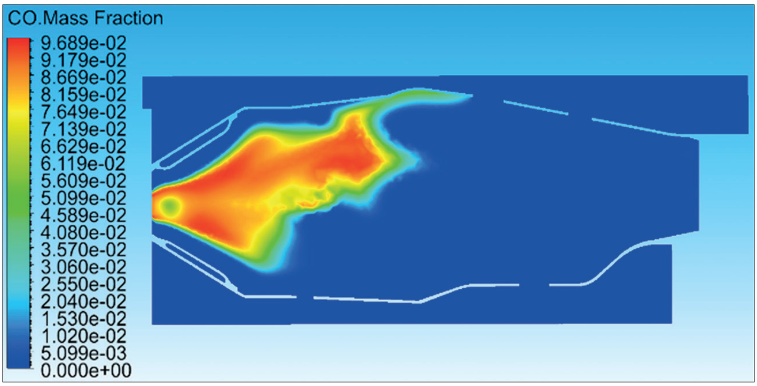


Figure 10.
Total pressure distribution [the authors]

Figure 11 demonstrates the distribution of the gases which are CO_2, CO, and O_2. These gases especially at the exhaust are one of the main and critical components to be taken as a reference for future research because of the impact of these gases on the environment and air quality.





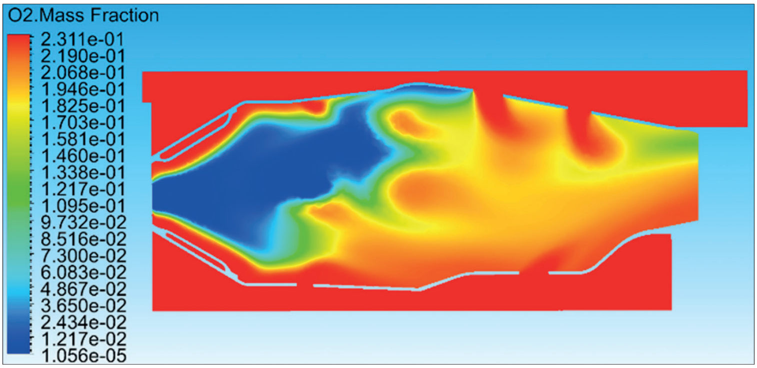


Figure 11.
Combustion gases emission distribution [the authors]

Thermal NO_x accounts for over 80% of all NO_x, therefore a thermal NO_x prediction is a good initial indicator of whether there are any major emission concerns with the design [19]. And as shown in Figure 12, the thermal NO_x follows the high temperatures.

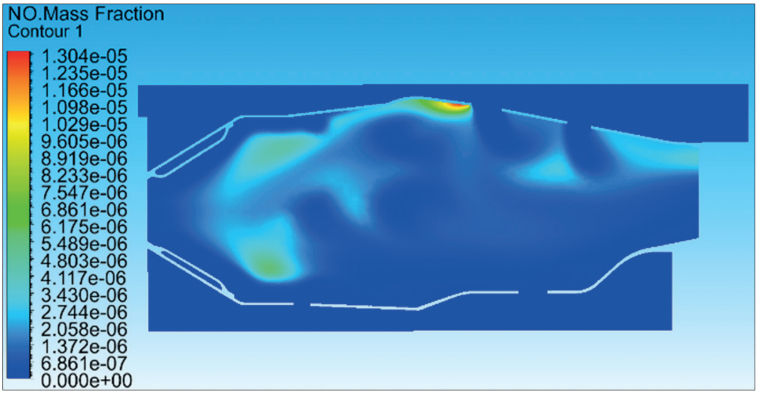


Figure 12.
Thermal NO_x prediction [the authors]

According to Table 2 the pressure recovery factor and averaged outlet temperature are slightly different than the previous study despite the fact that all boundary conditions are nearly the same. The differences are negligible. Most probably the reason is the different cell sizes and configurations where smaller element sizes were used in this study for a higher resolution mesh.

Table 2.
Comparison for verification [the authors]

	Parameters from this study [the authors]	Parameters from [5]
Pressure recovery factor	0.948	0.947
Averaged outlet temperature	1135.3 [K]	1136.97 [K]
Number of mesh elements	28,638,128	7,503,619

Conclusion

This paper presented a detailed Computational Fluid Dynamics (CFD) case study and analysis of the combustion process and gas emissions in the TKT-1 academic turbojet engine, with a focus on understanding the internal fluid dynamics, temperature distribution, pressure recovery factor, and distribution of the gases, which are O_2, CO, CO_2, and NO_x. The results of this investigation give significant insight into both the thermodynamic performance of the engine and its environmental footprint.

The temperature and total pressure distribution were highlighted. Since the turbine distribution parameters are critical not only for engine efficiency but also for the airworthiness of the turbine components, any new SAF mixture and green solution must obtain the same characteristics with the only difference being the ratios of the combustion chamber gases.

The results of this simulation are going to be a key component in further investigation and research by comparing the same parameters with the ones obtained by using different samples and mixture rates of SAF.

In conclusion, this investigation with the help of CFD modelling will play a leading role in advancing the optimisation of SAF mixtures when used in turbojet engines like the TKT-1. By providing detailed insights into the combustion process, temperature distribution, and gas emissions, the findings of this research contribute to ongoing efforts to improve the efficiency and environmental performance of jet engines. With continued advancements in computational methods and experimental validation, there is great potential for achieving cleaner, more efficient systems that meet the ongoing demands and needs of the modern aviation society and aeronautical developments.

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A TKT-1 tudományos sugárhajtóműben kialakult égési folyamat CFD-elemzése

Az égés bonyolult, kémiai reakció által kiváltott folyamat, amelyben a tüzelőanyag a levegőben lévő oxidálószerrel, általában oxigénnel egyesülve hőt termel. Az égés vizsgálata fontos az energiahatékonyság növelése szempontjából, és kulcsfontosságú eleme a további zöldebb megoldásoknak és környezetbarátabb fejlesztéseknek. A CFD-modellezés segítségével világosabb vizualizáció és a termikus tulajdonságok jobb megértése tárható fel. Ezeknek a speciális termikus *tulajdonságoknak a megértése lehetővé teszi a különböző tüzelőanyag-típusok pontos és hatékony összehasonlítását. E cikk célja, hogy modellezze az égést egy TKT-1 kísérleti gázturbinás hajtóműben fosszilis szabványos tüzelőanyagokkal, és összegyűjtse az égési kibocsátási paramétereket, hogy megfelelő összehasonlítást tudjon végezni ugyanezzel a folyamattal fenntartható tüzelőanyagok alkalmazása esetén.*

Kulcsszavak: *CFD-vizsgálat, égésszimuláció, égéstér-gázkibocsátás, TKT-1 égéstér-modellezés, fosszilis tüzelőanyag, fenntartható tüzelőanyag*

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