Numerical Evaluation of the Equilibrium Combustion Model in Methane Microturbines

Numeryczna ocena modelu równowagowego spalania w mikroturbinach metanowych

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Today when preparing a CFD study, there is a need to make a compromise between the results accuracy (applied models) and the computational cost. In this study the non-premixed equilibrium combustion model is assessed by a comparative numerical method, when applied to diffusion type gas microturbine combustor methane powered. In order to make it, a diffusion type gas microturbine combustor methane powered simulation was done twice, using one time the non-premixed equilibrium combustion model and second time the steady diffusion flamelet combustion model (with the use of Gri-Mech 3.0 mechanism), which is suitable for this specific application. The thermal operation parameters of both simulations were compared and their analysis shown that equilibrium model permits to obtains accurate thermal results, compared to more complex and accurate combustion model as the steady diffusion flamelet model.

Keywords: Gas Microturbine; Diffusion Type Combustor; Combustion Models; CFD; Gri-Mech 3.0.

Współcześnie, podczas przygotowywania badań CFD, istnieje konieczność znalezienia kompromisu między dokładnością wyników (zastosowanymi modelami) a kosztem obliczeniowym. W niniejszym badaniu model spalania równowagowego typu dyfuzyjnego został oceniony metodą porównawczej analizy numerycznej, przy zastosowaniu go do dyfuzyjnej komory spalania mikro turbiny gazowej zasilanej metanem. Aby tego dokonać, przeprowadzono dwukrotnie symulację dyfuzyjnej komory spalania: raz z wykorzystaniem równowagowego modelu spalania dyfuzyjnego, a drugi raz z użyciem modelu spalania dyfuzyjnego opartego o płomyki („flamelet" z j. ang. – z wykorzystaniem mechanizmu reagowania Gri-Mech 3.0), który jest odpowiedni dla tego rodzaju zastosowań. Porównano cieplne parametry pracy obu symulacji, a ich analiza wykazała, że model równowagowy pozwala uzyskać bardzo zbliżone wyniki (a zatem wiarygodne) w porównaniu z bardziej złożonym i precyzyjnym modelem spalania, jakim jest model spalania dyfuzyjnego opartego o płomyki.

Słowa kluczowe: mikro turbiny gazowe, dyfuzyjne komory spalania, modele spalania, CFD, Gri-Mech 3.0.

Introduction

In last decades, the evolution of computer calculation capacities permitted to develop CAE – type programs (Computer Aided Engineering). The aim of the CAE programs is to perform simulations using mathematical and physical models at various levels of precision. One of the most important applications of the CAE type tool is the CFD field (Computational Fluid Dynamics), permitting the simulation of flow phenomena, even taking into account the combustion. There is a need here to differ the CAE tools and the mathematical and physical models. The CAE tools are the implementation of mathematical and physical models into computer environments. The mathematical and physical models used in CAE are a set of models permitting to describe various phenomena occurring in real life. The most of this models were known even before the computers era. The apparition of powerful computers permitted to use these models, at various degrees of exactitude, to perform simulations. The models used in CAE are still enhanced, by continuous studies permitting to compare the CAE results and real phenomena. Today, the next CAE tools can be cited as example: Ansys, Fluent, Abaqus, OpenFoam ect. The use of these CAE tools permitted first to reduce the products elaboration time and funds reducing the number of performed prototypes. Then, the CAE tools permitted to discover and/or understand phenomena by the deep analysis of good quality simulations [1, 2]. CAE tools permit to be more efficient and economical in terms of products development and in physical phenomena better understanding.

The gas microturbines are devises that are widely used in various applications: in aviation to power drones, in the automotive industry as car's range extenders (e.g. Jaguar CX75), in the energy industry as electrical (and heat) generators. Gas microturbines present many advantages, such as low noise level, cheap design and operation, low emissions, large type of fuel applicability, etc. These criteria are the reason for the gas microturbine devices wildly use. [3] The gas microturbines are devices that are often equipped of diffusion combustion

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chambers. The diffusion combustor are older technologically solutions, in which the oxidizer and fuel are supplied separately. In this kind of combustor the combustion is non-premixed, evolving from rich to leam mixture, permitting good flame stability and safe combustor operation. This devices can be powered by various fuel (jet-A, gasoline, petrol, waste gas, methane, ect.), but one of the most popular fuel is methane.

According to the above, it must be denoted that actually many gas microturbines methane powered are designed and that the one of most efficient design tools is the CFD domain. In order to enhance the design process of these devices, there is a need to use CAE tools permitting to model the physical phenomena as: fluid flow, combustion, and radiation [3]. One of the most popular CFD tool able to make it is Ansys Fluent [4]. As exposed above, the applied mathematical and physical models can be implemented at various degrees of exactitude.

As exposed before, the diffusion type combustors are widely used in the gas microturbines. In order to numerically analyse these kind of devices, there is a need to use a non-premixed combustion model, applied to CFD methods. The often applied combustion models are the finite-rate chemistry with the Eddy Dissipation Model (EDM) [5 – 8] or the Eddy Dissipation Concept (EDC) [9 – 13], Composition PDF Transport [14 – 16] and the steady diffusion flamelet model [17 – 20].

Eddy-dissipation model – The model allows for the calculation of the reaction rate based on a simple combustion mechanism (preferably two-step mechanism), taking turbulence into account. The model does not support the simulation of detailed combustion mechanisms, which results from the fact that it does not consider chemical kinetics and assumes that all reactions proceed at the same rate – an incorrect assumption as the number of reactions in the combustion mechanism increases. The model is of general-purpose use for combustion process modelling; it is computationally efficient but does not support work with complex combustion kinetics, which limits its applicability and accuracy.

Eddy-dissipation-concept (EDC) model – The model is a significantly improved and extended version of the Eddy-Dissipation Model. It accounts not only for turbulence in the calculations but also includes chemical kinetics. This allows for the implementation of detailed combustion mechanisms. The model is relatively accurate and can be considered a general-purpose model for combustion process simulations. Since it solves transport equations for each species during processing, it is highly demanding in terms of computational resources, which can significantly increase computation time.

Composition PDF Transport – It is an alternative model to the Finite-Rate Chemistry approach, in which solving the averaged species equations is replaced by computing the derivative of these equations at a selected location and approximating them using a probability density function (PDF). The PDF has a dimension of N+1, where N is the number of species included in the combustion mechanism. This approach allows for bypassing highly nonlinear reaction rates. The model offers good accuracy and is also considered a general-purpose model for combustion process simulations. Unfortunately, it is also computationally demanding and is characterized by long computation times.

The Non-Premixed Model approach is based on determining mean temperature, density, and mass fractions of chemical species using the mixture fraction and its variance. This model takes into account the influence of turbulence on combustion. Equilibrium Model – the model assumes a state of chemical equilibrium, which is not entirely accurate for reactions that, in reality, do not reach equilibrium. Steady Diffusion Flamelet Model – this model allows for the inclusion of detailed chemical combustion kinetics (the chemistry can be in non-equilibrium state, but close to). The selected combustion model is computationally efficient.

The main limitations of the Equilibrium combustion model compared to the Flamelet model are listed below:

- Equilibrium model may not predict intermediate species (CO, NOx, etc.) as accurately as Flamelet model, that resolves finite rate kinetics making possible to capture pollutant formation and incomplete combustion, especially in regions with rapid mixing, quenching, or flame extinction;
- Equilibrium model assumes the entire domain as uniform equilibrium products, while Flamelet model retains spatial gradients across the flame front (thickness, temperature, radical distribution);
- Equilibrium model predicts a stable flame in presence of fuel and oxidizer, while Flamelet model takes into account the scalar dissipation rate, making possible to predict local extinction and reignition in turbulent flows;
- Equilibrium model assumes instantaneous mixing and chemistry while Flamelet model treats mixing (scalar dissipation rate) and chemistry;
- Equilibrium model results are insensitive to flow strain, turbulence, and mixing rates compared to Flamelet model that takes these phenomena into account;
- Equilibrium generally provides adiabatic flame temperature, while Flamelet model includes heat losses and finite-rate effects, leading to more realistic temperatures.

Based on the above, it can be stated that the selection of combustion model is a compromise between result accuracy and computational time. The Non-Premixed Equilibrium combustion model is a model that assumes the combustion occurs in the chemical equilibrium. In the gas microturbine, the combustion time is reduced by the short length of the combustion chamber. It means that the combustion mays be not on its chemical equilibrium. At the same time, the combustion in gas microturbine is strongly turbulent, due to its design. As the turbulence of a flame increases, its chemical rate increases. This phenomenon could permit to move closer to the chemical equilibrium. Taking into account both phenomena (short length and high turbulence level), the combustion in gas microturbine devices seems not to be too far from the equilibrium combustion, making this model partially applicable.

The aims of this paper is to compare the Non-Premixed Steady Diffusion Flamelet model, known to be accurate for gas microturbine combustion modelling, with the Equilibrium model, rarely (not) used for this purpose, under the thermal aspect. The CFD study will be conducted using a self-designed combustion chamber for methane powered gas microturbine of about 40 kW of mechanical output power.

After calculations, the two models thermal proprieties will be compared. As the Non-Premixed Steady Diffusion Flamelet model is known to provide accurate results, if its results will be similar to these of the Non-Premixed Equilibrium, it will mean that the Non-Premixed Equilibrium model is suitable and accurate for methane powered gas microturbine diffusion type combustors. In this study, the thermal proprieties will be checked.

If the use of the Non-Premixed Equilibrium model will be positively assessed in this specific application, it will permit to engineers and scientists to perform easier and using more basic combustion model for preliminaries thermal analyses of combustors. It will permit to open new applications to the studied combustion model.

Else, the paper will permit to prevent to not use this model for these or similar purposes. According to literature review, this aspect of the non-premixed equilibrium combustion model was not yet studied.

Study case combustor and operating conditions

The announced research need to be performed on a methane powered gas microturbine which operation parameters are defined. To respond to this demand, a gas microturbine combustion chamber was calculated, designed and 3D model was created, using SolidEdge CAD tool [21]. This combustor is designed for a 40 kW output mechanical gas microturbine. The combustion chamber operation parameters are listed in Table 1. This device design is presented in Figure 1. In the past, this combustor was already used in other research [3, 22].

Table 1. Operation parameters of the used methane powered gas microturbine

Operation parameters	Combustor inlet section	Combustor outlet section
p^* [kPa]	325	312
p [kPa]	307	301
T^* [K]	433	1185
T [K]	426	1175
$\dot{m} = 0.251\ \frac{kg}{s};\ c_s = 0.004874\ \frac{kg}{s}$		

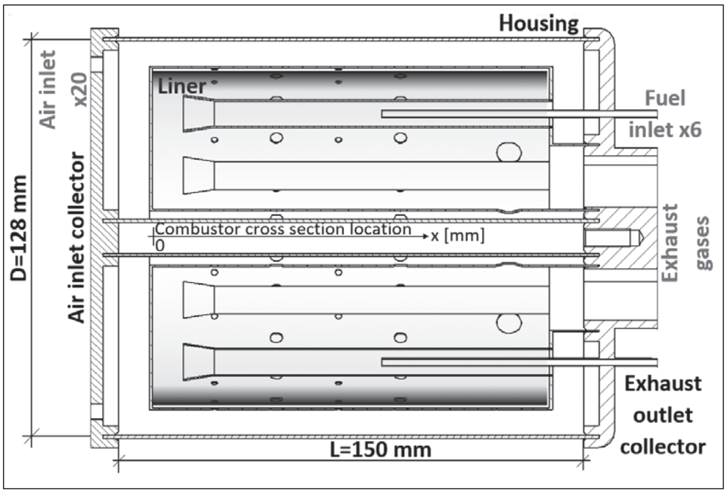

Figure 1. Methane powered gas microturbine combustor designed for CFD research

Numerical methods

Calculation domain

The 3D model of combustion chamber was created using SolidEdge software [21], while its waterflow model, enabling numerical calculations, was generated based Ansys Fluent-Meshing software [4]. The generation of computational mesh is one of most important steps in conducting numerical studies of combustion chambers. To generate a mesh of the combustion chamber, tetrahedral elements are often used, as they have already proven accuracy in numerical calculations of combustors in the past [18, 19, 25]. The use of this element allows for the filling of highly complex computational domain geometries while maintaining acceptable mesh quality parameters (Skewness, Orthogonality, and Aspect Ratio). Recently, significant efforts have been made to develop numerical meshes build from polyhedral elements. Similar to tetrahedral elements, polyhedral elements allow for obtaining good computational results while simultaneously improving mesh quality [26, 27]. Therefore, polyhedral elements were selected for building the computational mesh.

Firstly, the mesh cells with a maximum length of 0.8 mm were applied for this research. Then, the volume mesh was generated and improved by applying the value of 0.45 as the cell desired orthogonal quality. Finally, five boundary layers were generated in order to limit the Y+ value at less than 300. According to the literature [18, 25], the obtained calculation domain mesh is sufficient to provide reliable results. Table 2 shows the quality parameters of the obtained mesh system, while Figure 2 presents the mesh of the calculation domain.

Table 2. Combustor mesh quality parameters

Number of cells [millions]	Maximum aspect ratio [-]	Maximum skewness [-]	Minimum orthogonal quality [-]
5.8	38.3	0.895	0.435

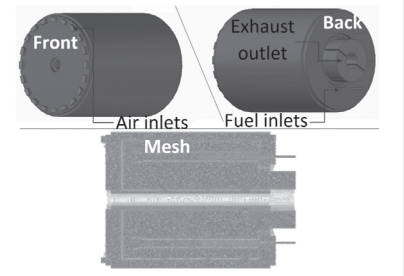

Fig. 2
Combustor calculation domain view

Mathematical models

Numerical studies of a 3D combustion chamber were carried out using Ansys Fluent software [4]. The following physicochemical processes were modelled: turbulent flow, non-premixed combustion in the gas phase, and heat transfer by radiation within the computational domain. These key phenomena were modelled to obtain accurate comparative numerical results.

Model of the turbulent flow

For the flow description, the RANS (Reynolds-Averaged Navier-Stokes) approach was chosen, which is based on the averaged Navier-Stokes equations. To describe turbulence, the Realizable k-ε model was applied, which is widely used in many industrial and similar applications. This model allows for flow modelling with acceptable accuracy at a low computational cost. For near-wall flow, the "Enhanced Wall Treatment" approach was applied. This allows computing the flow in the near-wall region when the normalized distance from the wall is less than or equal to unity ($y^+ \le 1$), or by using a near-wall function called the "Enhanced Wall Function" ($y^+ > 1$). This is an optimal solution when the phenomena occurring in the near-wall region are not critical, as is the case in this computational study.

Model of the radiation

In the investigated combustion chamber, the dominant heat transfer mechanism is radiation. To describe this phenomenon, the Discrete Ordinates (DO) model [18] was used, which treats the computational domain as a mixture of gray gases. The two main compounds that affect significantly absorption and emission capabilities in the combustion zone (within the combustion chamber) are carbon dioxide and water steam. To accurately model the mentioned properties of the gas mixture, the Weighted Sum of Gray Gases Model (WSGGM) was selected. This model accounts for the radiative properties of the flue gas components based on experimental studies [26] and is widely applied in numerical calculations of combustion chambers. The chamber walls were assumed to behave as blackbody surfaces [27].

Models of the non-premixed combustion

Both, the Non-Premixed Equilibrium Combustion Model and the Steady Diffusion Flamelet Combustion Model assume the use of a "Look-up Table" (generated during pre-processing step) and several calculated coefficients during processing (such as the mean mixture fraction and its variance, the mean scalar dissipation rate, and the mean enthalpy) to retrieve combustion process mean parameters (species mass fraction, temperature, and density).

Non Premixed Equilibrium Combustion Model

The instantaneous combustion parameters, Φ_i, such as species mass fraction, temperature, and density, are calculated based on the available chemical species included in the computations, the general laws of chemical reactions, the local enthalpy level (in the case of non-adiabatic process), and the availability of oxidizer and fuel, which are described using the mixture fraction. The available chemical species and the enthalpy levels are defined during the pre-processing step by specifying the fuel and oxidizer species and partially by their temperatures. The mixture fraction takes values from 0 (pure oxidizer) to 1 (pure fuel). Based on this set of variables and their ranges, together with the general chemical reaction laws, the instantaneous values of the parameters describing the combustion process at equilibrium, Φ_i, are calculated for each state, where $\Phi_i = \Phi_i(f, H)$. Here, a non-adiabatic Beta-type probability density function (PDF) $p = p\,(f,\ H)$ is used.

In order to simplify the calculations, the next assumption is done: the enthalpy fluctuations are independent of the enthalpy level. This assumption conducts to the use of mean enthalpy instead of the instantaneous enthalpy. Because of that, it can be noted that $\Phi_i = \Phi_i(f, \overline{H})$ and $1 = p(f)$.

The integration of the instantaneous parameters Φ_i with the probability density function (PDF) p allows for the generation of the Look-up Table (in the case for the Non-Premixed Equilibrium Combustion Model) through the following equation (3.1):

$$\overline{\Phi}_i = \int \Phi_i\left(f, \overline{H}\right) p(f)\,df \qquad (3.1)$$

The result of these calculations is the generation of a database that can be used during the processing step, using the values of the following parameters: $\overline{f}$, $\overline{f'^2}$ and $\overline{H}$, calculated using the appropriate transport equations during processing step. This Look-up Table returns the mean values of parameters describing the combustion process (mass fraction of the *i*-th species, density, and temperature): $\overline{Y}_i$, $\overline{\rho}$ oraz $\overline{T}$.

Steady Diffusion Flamelet Combustion Model

The instantaneous combustion parameters Φ_i, such as species mass fraction, temperature, and density, are calculated based on the combustion mechanism implemented for the calculations (in this study case, GRI-Mech 3.0), the availability of oxidizer and fuel described by the mixture fraction and its variance, as well as the scalar dissipation rate. The enthalpy is also to be taken into account when a non-adiabatic system is treated. Based on this set of variables and their value ranges, selected mechanism, the instantaneous parameters describing the combustion process in a state deviating from equilibrium (expressed by the scalar dissipation rate) are calculated, Φ_i, where $\Phi_i = \Phi_i(f, \chi, H)$. Each of these χ states is referred to as a "flamelet". To generate the flamelet structure parameters for each scalar dissipation rate χ, equations (3.2) for each species and one energy equation (3.3) are solved:

$$\rho \frac{\partial Y_i}{\partial t} = \frac{1}{2} \rho \chi \frac{\partial^2 Y_i}{\partial f^2} + S_i \qquad (3.2)$$

$$\rho \frac{\partial T}{\partial t} = \frac{1}{2} \rho \chi \frac{\partial^2 T}{\partial f^2} - \frac{1}{c_p} \sum_i H_i S_i + \\ + \frac{1}{2c_p} \rho \chi \left[\frac{\partial c_p}{\partial f} + \sum_i c_{p,i} \frac{\partial Y_i}{\partial f} \right] \frac{\partial T}{\partial t} \qquad (3.3)$$

The database of flamelets used in this combustion model was generated based on the GRI-Mech 3.0 combustion mechanism [28]. This mechanism includes 53 chemical species and 325 chemical reactions. Appropriate sets of flamelets (and later the Look-up Table) were generated for numerical combustion calculations. Air was simplified to a mass fraction of 23% oxygen and 77% nitrogen. In order to simplify the calculations, the next assumption is done: the enthalpy fluctuations are independent of the enthalpy level. This assumption conducts to the use of mean enthalpy instead of the instantaneous enthalpy. Because of that, it can be noted that: $\Phi_i = \Phi_i(f, \chi, \overline{H})$ and $p = p(f, \chi)$.

In order to generate the Look-up Table, the instantaneous parameters of the combustion process, denoted by Φ_i, must be integrated with the probability density function (PDF) p. The integration is performed using the following relation (3.4):

$$\overline{\Phi}_i = \iint \Phi_i\left(f, \chi, \overline{H}\right) p\left(f, \chi\right) df\,d\chi \qquad (3.4)$$

The result of the calculations is the generation of a database (Look-up Table) of the following parameters: $\overline{f}$, $\overline{f'^2}$, $\overline{\chi}$ and $\overline{H}$. The Look-up Table returns the parameters mean values describing the combustion process (mass fraction of the i-th species, density, and temperature): $\overline{Y}_i$, $\overline{\rho}$ oraz $\overline{T}$.

Boundary conditions

After the mesh generation, the implementation of the mathematical models, the boundary conditions were applied, as described in the next table 3.

Table 3. The boundary conditions

Designation of the boundary condition	Type of boundary condition	Parameters
Air inlet	Mass Flow Inlet	Mass flow=0.251 kg/s; Turbulent Intensity=15 %; Turbulent Viscosity Ratio= 10; Total Temperature=433 K; Mean Mixture Fraction= 0; Mixture Fraction Variance= 0;
Fuel inlet	Mass Flow Inlet	Mass flow=0.004874 kg/s; Turbulent Intensity=15 %; Turbulent Viscosity Ratio= 10; Total Temperature=300 K; Mean Mixture Fraction=1; Mixture Fraction Variance=0;
Exhaust	Pressure Outlet	Static Pressure=0 Pa; Turbulent Intensity=15 %; Turbulent Viscosity Ratio=10; Backflow Total Temperature=1200 K; Mean Mixture Fraction=0; Mixture Fraction Variance=0;
Wall	Wall	Stationary Wall; No Slip; No Heat Exchange; Internal Emissivity=1; Opaque Wall; Diffuse Fraction of Radiation=1;
Operating conditions	-	Operating pressure=301 kPa, Gravity off;

Results and Discussion

Gas microturbine main operation parameters

When dealing with a gas microturbine combustion chamber, the most important operation parameters are the total pressure drop through the device and the total temperature at the outlet. Additionally the outlet static temperature will be treated. The total pressure drop was calculated using the equation 4.1. The operation parameters are presented in the table 4. As it can be seen the relative differences between both combustion models are very small.

$$\Delta p^* = \frac{p_2^* - p_3^*}{p_2^*} \cdot 100 \qquad (4.1)$$

Table 4. Combustor main operation parameters

	Non Premixed Equilibrium Combustion Model	Non Premixed Steady Flamelet Model
Δp* [%]	10.08	10.09
T3* [K]	1231	1241
T3 [K]	1217	1229

According to the presented results, the total pressure drop occurring in the combustion chamber is very similar for both combustion models: 10.08 % for the non-premixed equilibrium combustion model and 10.09 %. The relative difference between both results is about 0.06 %, which is neglectable. The calculations have shown that the choice of discussed combustion models have no impact on the total pressure drop. This is a positive observation; the total drop pressure is not impacted when using simpler combustion model (the non-premixed equilibrium combustion model) regarding a more complex model (steady diffusion flamelet combustion model).

As in the case of the exhaust gases total temperature, this parameter is not impacted regarding the combustion model choice. The total temperatures are very closes: 1231 K for the equilibrium combustion model and 1241 K for the steady diffusion flamelet combustion model. The exhaust total temperature is higher in the flamelet combustion model compared to the equilibrium combustion model. On the one hand, in the equilibrium combustion model, the combustion is assumed to be at the equilibrium state – the fuel would be better consumed, while in the flamelet model, where the combustion occurs in a state near to equilibrium but out of this one, which mays lead to less complete combustion of the fuel. On the other hand, the turbulence phenomena, the fuel and oxidizer availability, and combustion models differences make the interpretation of these phenomena and results extremely complex, more complex than simple higher or lower fuel transformation degree. These both observations make the difference of maximum temperature, at exhaust, for both combustion models, not really foreseeable. The exhaust total temperatures in both combustion models are very closes: 0.82 %, which can be neglected in primary engineering and scientific studies. This reduced difference, in term of the exhaust total temperature, comes to confirm the idea that the high turbulence of the flow in the combustion chamber lead to a faster combustion, which makes the results from both combustion models closes. This is a positive observation; the exhaust total temperature is not impacted when using simpler combustion model (the non-premixed equilibrium combustion model) regarding a more complex model (steady diffusion flamelet combustion model).

The temperature parameters analysis

The temperature in whole liner volume

The mean and maximum static temperature in the whole liner volume will be presented and discussed. The analysis of these parameters, especially the maximum combustion temperature, is crucial from a material heat resistance of the combustion chamber structure point of view. These parameters are presented in table 5.

Table 5. The mean and maximum temperature in whole combustor liner regarding the selected combustion model

Non Premixed Equilibrium Combustion Model		Non Premixed Steady Flamelet Model		Models parameters relative diference [%]	
Tmed [K]	Tmax [K]	Tmed [K]	Tmax [K]	Tmed [K]	Tmax [K]
757	2266	755	2297	0.26	1.37

First, the maximum volumetric static temperature is considered. In both combustion models, the peak temperature inside the liner is very similar: 2266 K for the non-premixed equilibrium model and 2297 K for the steady diffusion flamelet model, a relative difference of only 1.37%. This agrees with the small temperature difference observed at the combustor outlet. Local effects—fuel/oxidizer availability, inlet conditions, and turbulence—explain the minor variations between models. Since the maximum temperatures are nearly identical, the choice of model is not critical for estimating this parameter, and the simpler equilibrium model is sufficient for initial analyses.

Second, the mean volumetric static temperature also shows negligible differences: 757 K for the equilibrium model and 755 K for the flamelet model (0.26% difference). This indicates that, despite their different assumptions—chemical equilibrium vs. finite-rate chemistry—both models describe the combustion similarly under the highly turbulent and geometrically constrained conditions of a gas microturbine combustor. High turbulence accelerates chemical reactions, pushing the system closer to equilibrium even when residence times are short. Thus, both models remain applicable, and the simpler equilibrium model is adequate for preliminary evaluation of mean volumetric static temperature in microturbine combustion chambers.

The temperature maps analysis in the liner

The mean and maximum static temperature and the static temperature uniformity index, through selected combustor axial sections in the whole combustion chamber, will be presented and discussed. The static temperature uniformity index is calculated applying the equation 4.2. The axial sections of the combustor are shown on the figure 3. The analysis of these parameters, especially the maximum combustion temperature, is crucial from a material heat resistance point of view. These parameters are presented in table 6, while their differences between both combustion models are presented on figure 4.

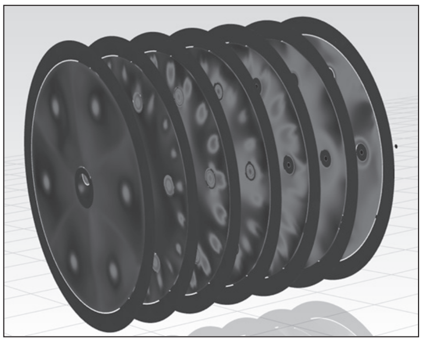

Figure 3.
Visualisation of the cross sections studied of the combustor

Table 6. The mean and maximum temperature, and its uniformity index, in combustor cross-sections regarding the selected combustion model

	Non Premixed Equilibrium Combustion Model			**Non Premixed Steady Flamelet Model**			**Models parameters relative diference [%]**		
X [m]	**Tmed [K]**	**Tmax [K]**	**UIT [-]**	**Tmed [K]**	**Tmax [K]**	UIT [-]	Tmed [%]	Tmax [%]	UIT [%]
0.00	859	2175	0.817	836	2234	0.819	2.73	2.69	0.29
0.01	835	2184	0.815	836	2267	0.817	0.21	3.77	0.18
0.02	889	2169	0.812	885	2258	0.814	0.48	4.11	0.24
0.03	845	2215	0.811	844	2281	0.813	0.19	2.99	0.26
0.04	927	2200	0.794	930	2253	0.793	0.28	2.38	0.19
0.05	976	2189	0.804	984	2237	0.802	0.86	2.21	0.26
0.06	952	2203	0.805	962	2261	0.803	1.04	2.66	0.22
0.07	930	2234	0.799	939	2274	0.798	1.07	1.78	0.16
0.08	962	2205	0.786	973	2265	0.783	1.18	2.75	0.45
0.09	987	2205	0.804	997	2261	0.803	0.98	2.58	0.13
0.10	1007	2204	0.810	1020	2267	0.809	1.27	2.87	0.13
0.11	946	2219	0.781	970	2261	0.778	2.53	1.92	0.29
0.12	998	2213	0.793	1019	2275	0.793	2.10	2.78	0.09
0.13	1006	1876	0.777	1020	1857	0.775	1.37	1.03	0.31
0.14	1199	1691	0.945	1209	1698	0.947	0.83	0.41	0.21
0.15	1200	1631	0.951	1210	1651	0.953	0.82	1.21	0.19

$$UI^{plane}_{area} = 1 - \frac{\sum_{i=1}^{N}\left[\left(\left|T_{facei} - T_{average}\right|\right)\cdot A_i\right]}{2\cdot T_{average}\cdot\sum_{i=1}^{N}\left[A_i\right]} \quad (4.2)$$

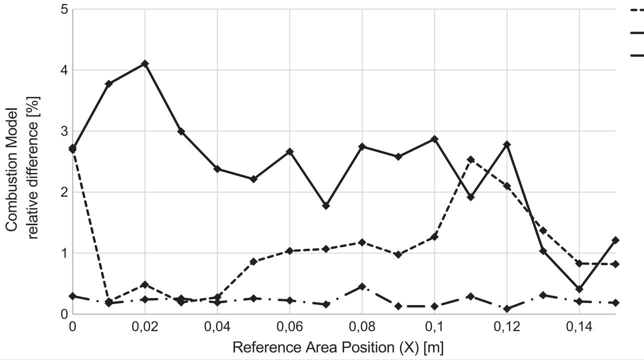

Figure 4. Combustor thermal operation parameters, through axial cross-section, relative differences between applied combustion models

The maximum combustion static temperature varies along the combustor depending on local conditions. For both models the values are close: 1631–2234 K for the non-premixed equilibrium model and 1651–2281 K for the steady diffusion flamelet model. The relative differences range from 0.41% to 4.11%—small, though not entirely negligible. The flamelet model generally predicts slightly higher peak temperatures, with one local exception at X = 0.13.

These differences arise from local fuel–oxidizer availability, thermal and pressure conditions, and turbulence levels, combined with the inherent calculation differences between the models. Still, the peak temperatures remain sufficiently close to consider both models acceptable for preliminary engineering or scientific analyses. Typically, the simpler equilibrium model yields slightly lower maxima—up to about 4%—but such deviations remain tolerable. Therefore, the choice of combustion model is not critical for estimating the maximum combustion static temperature, and the simpler non-premixed equilibrium model is adequate for initial studies.

The mean combustion static temperature will be then treated. The mean static temperature evolves from section to section, depending on the local environment conditions. These temperatures are very closes for both combustion models: range from 835 K to 1200 K for the non-premixed equilibrium combustion model, versus a range from 836 K to 1210 K for the steady diffusion flamelet model. The relative difference for this parameter evolves from 0.19 % to 2.73 %, which is low difference, quasi-neglectable. Reversely to maximum combustion static temperature, there is no rule in terms for which combustion model the mean combustion temperature will be higher or lower than the second one. It means that the phenomena occurring inside of the combustor, permit to obtain similar combustion description when applying both combustion models. The Non-Premixed Equilibrium combustion model assumes that the combustion occurs in the chemical equilibrium, while the steady diffusion flamelet model assumes the reaction rate importance in combustion process. In the gas microturbine combustors, the combustion time is limited; it would mean that the combustion mays be not on its chemical equilibrium, leading to the use of steady diffusion flamelet model. At the same time, the combustion in gas microturbine is strongly turbulent. As the turbulence of a flame increases, its chemical rate increases too; this observation could permit to move closer to the chemical equilibrium, leading to the use of non-premixed equilibrium combustion model. Taking that into account, the combustion in gas microturbine devices seems not to be too far from the equilibrium combustion, making both models applicable. The behaviour of the mean combustion static temperature comes to support this thesis. In the context of the mean combustion static temperature, the performed observation is positive regarding the issue of these research – the choice of the combustion model is not of crucial importance regarding the combustion mean static temperature. A simpler combustion model can be applied despite of more complex combustion model, when analysing initially the mean static temperature.

The combustion static temperature uniformity index varies along the combustor but remains almost identical for both models: 0.777–0.951 for the non-premixed equilibrium model and 0.775–0.953 for the flamelet model. The relative differences (0.09–0.45%) are negligible. Its behaviour mirrors that of the mean combustion static temperature discussed earlier, and no additional phenomena were noted. This confirms again that the choice between the two combustion models has no significant impact on preliminary thermal analysis of gas microturbine combustors.

Calculation time comparison between both applied models

The calculations for both combustion models were conducted on the same computer. This hardware operation parameters are listed below:

- Processor: Intel(R) Core(TM) i9-14900K 3.20 GHz; 24 physical cores: 8 Performance-cores (P-cores) and 16 Efficient-cores (E-cores);
- Ram: 128 GB.

During operation, only 10 cores were dedicated for the Fluent calculations. The calculation time for the Equilibrium model was of 61380s, while for the Flamelet model it was 80220s. The use of the more complex model (Flamelet model), compared to the Equilibrium model, provokes the calculation time increases of about 30%. This value is not yet neglectable, which is also an important, looked for, advantage of using the simpler combustion model despite of the more complex one, for the thermal initial calculations.

Conclusions

The present studies permitted to compare the non-premixed equilibrium combustion model to the steady diffusion flamelet combustion model, applied to a gas microturbine diffusion type combustion chamber methane powered. Three groups of operation parameters where studied: the main operation parameters, the thermal operation parameters and the calculation time.

In terms of the main operation parameters, the total pressure drop and exhaust gas total temperature were assessed. Additionally, the exhausts static temperature was also analyzed. The present studies showed that the choice of the discussed combustion models has no impact on these main operation parameters, in this specific application case, described before.

In terms of the thermal operation parameters, the next parameters were analyzed: mean and maximum combustion volumetric static temperature, maximum and mean combustion static temperature and its uniformity index. The present studies showed that the choice of the discussed combustion models has no impact on these thermal operation parameters, in this specific application case, except one: the maximum combustion static temperature; the application of the non-premixed equilibrium combustion model leads to lower values of this parameter, reaching even about 4 %.

In terms of the hardware calculation time, the use of the more complex model (Flamelet model) leads to a calculation time extension of about 30% compared to the use of the simpler model (Equilibrium model). This value is not negligible and constitute an advantage when primary thermal calculations are conducted.

According to the above, the choice of simpler combustion model (the non-premixed equilibrium combustion model) despite of more complex combustion model (the steady diffusion flamelet model) has no crucial impact on the thermal operation parameters when applied to a methane powered gas microturbine diffusion type combustor. Simpler model can be used for thermal initial studies in this specific case.

Nomenclature

A_i – area of facet defining analysed surface [m^2]
c_p – heat capacity at constant pressure [J/(kg.K)]
$c_{p,i}$ – mixture i-element heat capacity at constant pressure [J/(kg.K)]
c_s – methane (fuel) mass flow [kg/s]
f – mixture fraction [-]
$\overline{f}$ – mean mixture fraction [-]
$\overline{f'^2}$ – mixture fraction variance [-]
H – enthalpy [J/kg]
$\overline{H}$ – mean enthalpy [J/kg]
H_i – enthalpy of mixture i-element [J/kg]
$\dot{m}$ – air mass flow entering the combustor [kg/s]
p – static pressure [Pa]
p* – total pressure [Pa]
p(i,j,k...) – probability density function
p_2^* – total pressure at combustor's inlet [Pa]
p_3^* – total pressure at combustor's outlet [Pa]
Δp* – total pressure drop in combustor [%]
S_i – mixture i-element chemical reaction rate
S_m – source term due solely to transfer of mass into the gas phase from liquid fuel droplets or reacting particles
t – time [s]
T – static temperature [K]
T* – total temperature [K]
$\overline{T}$ – mean temperature [K]
T_{facei} – static temperature on i-th facet defining analysed surface [K]
Tmax – maximum static temperature [K]
Tmed – mean static temperature [K]
T3* – total exhaust temperature [K]
UI_{area}^{plane} – area averaged uniformity index [-]
UIT – static temperature area averaged uniformity index [-]
$\overline{Y}_i$ – mean mass fraction of the i-th species [-]
Y_M – represents the contribution of the fluctuating dilatation in compressible turbulence to the overall dissipation rate
ρ – density [kg/m^3]
$\overline{}$ – mean density [kg/m^3]
χ – scalar dissipation rate [1/s]
$\overline{\chi}$ – mean scalar dissipation rate [1/s]

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