# Numerical Investigation of a 7-Element GOX/GCH4 Subscale Combustion Chamber

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## Abstract

For future liquid rocket engines methane has become the focus of several studies on alternative fuels in the western hemisphere. At ArianeGroup numerical simulation tools have been established as a powerful instrument in the design process. In order to achieve the same confidence level for CH4/O2 as for H2/O2 combustion, the applied numerical models have to be adapted and validated against sufficient test data. At the Chair of Space Propulsion at the Technical University of Munich (TUM) several combustion chambers have been designed and tests at different operating points have been conducted. In this paper one of these subscale combustion chambers with calorimetric cooling and seven shear coaxial injection elements running on gaseous methane and oxygen is used to examine ArianeGroup's in-house tools for combustion chamber performance analysis.

## 1. Introduction

Current development programs in many space-faring nations focus on launchers utilizing a propellant combination of liquid oxygen (LOX) and liquid methane (CH4). In Europe, hydrocarbons have been identified as an alternative fuel in the frame of the Future Launcher Preparatory Programme (FLPP).<sup>14,23</sup> Major industrial development of methane / oxygen rocket engines is ongoing in the United States at SpaceX with the Raptor engine (staged combustion), at Blue Origin with the BE-4 engine (staged combustion) and in Europe at ArianeGroup with the Prometheus engine (gas generator). At ArianeGroup, concept studies of a full scale LOX/CH4 thrust chamber demonstrator in the 400 kN thrust range were initiated in 2007 and testing activites on the P3.2 test bench of the Deutsches Zenrum für Luft- und Raumfahrt (DLR) in Lampoldshausen, Germany, began in 2015. An overview on the current status of the thrust chamber demonstrator tests is given by Blasi and Häberle.<sup>1</sup>

The European development effort of propulsion systems for a next generation launcher is supported by national research programs. In Germany, fundamental research on methane / oxygen combustion is funded by the Deutsche Forschungsgesellschaft (DFG) within the Collaborative Research Center TRR40 on the topic of "Fundamental Technologies for the Development of Future Space-Transport-System Components under High Thermal and Mechanical Loads" (see also www.sfbtr40.de) and by the Bayerische Forschungsstiftung (BFS) within the project "Umweltfreundliche Treibstoffkombination LOX/Methan". The work on this paper was performed in the frame of both aforementioned projects in strong cooperation with the Chair of Space Propulsion at the Technical University of Munich (TUM) providing the experimental verification database.

## 2. Choice of Testcase

#### 2.1 Overview on Available GOX/GCH4 Test Data at TUM

The successful application of CFD tools to rocket thrust chambers requires a validation of simulation results with experimental data. At the Chair of Space Propulsion at TUM, several testbenches utilizing the propellant combination



Figure 1: Schematic View of the 7-Element Combustion Chamber

oxygen / methane are in use to increase the understanding of hydrocarbon combustion processes and to provide fundamental validation data for numerical tools.

For injection element characterization purposes, single element combustion chambers with both a circular and a square cross section based on a capacitively cooled hardware are operated, allowing for an an easy variation of injection elements, e.g. recess variations. Several publications by Celano et al.<sup>2,3</sup> and Silvestri et al.<sup>18,19,21</sup> present the hardware, the conducted experiments and their results in detail.

Additionally, two subscale multi-element combustion chambers with a capacitively and a water cooled hardware are currently in use. The first chamber has a rectangular cross section with five injection elements in one line allowing for a characterization of heatflux and temperature stratification perpendicular to the main flow direction. The latter multi-element combustion chamber has a circular cross section and seven injection elements. Hereby, the active cooling of the respective hardware allows for extended test durations ensuring steady state conditions. Furthermore, it enables the determination of the integral heat loads by measuring the coolant heat-up. Knab et al.<sup>6</sup> concluded that for a rocket combustion chamber with representative element-element and element-wall distances. Additionally, the operating conditions like combustion pressure and mixture ratio should match those of a full-scale rocket combustion chamber at TUM has both a representative injection element pattern and an operating point comparable to a mid-thrust engine and thus was chosen as a test case. While the chamber is currently operated with gaseous oxygen (GOX), a transition to liquid oxygen is foreseen to better match the injection conditions in state of the art large-scale rocket engines.

## 2.2 Description of the Test Specimen

The chosen multi-element combustion chamber has a circular cross section with an inner diameter  $d_{cvl} = 30$  mm and a contraction ratio  $\varepsilon_c = 2.5$ , resulting in a throat diameter  $d_t = 19$  mm. The total length l of the combustion chamber from faceplate to exit plane is 383 mm. It is designed for combustion chamber pressures of up to 100 bar and a maximum combustion temperature of 3600 K. The hardware is manufactured from oxygen free high conductivity copper (OFHC-Cu) and comprises of five water cooled segments of which four make up the cylindrical part of the combustion chamber and one contains the convergent divergent nozzle. A schematic view of the chamber layout is given in Figure 1. The first cylindrical segment has milled cooling channels with a rectangular cross section, comparable to the current cooling channel design in flight proven thrust chambers like Vulcain 2 or HM7B. Segments 2A, 2B and 3 feature drilled cooling channels, which are both cheaper and easier in the manufacturing process. The cross section of the cooling channels in the nozzle segment is rectangular, like in segment 1. The coolant water is routed in two cycles. The first cycle enters the distribution manifold on the upstream end of segment 1 and is routed through segments 1, 2A, 2B and 3 where it leaves segment 3 on the downstream end. The second cycle is solely used for the cooling of the nozzle segment. As injection element, a coaxial-shear element with a central GOX post and an annular GCH4 sleeve is used. For the current experiments the GOX post is mounted flush with the faceplate and possesses no tapering. The injection pattern is shown in Figure 2 and exhibits a central element on the chamber axis and six equally spaced elements on a concentric circle with a radius of  $3/2D_o$ . This ensures that the injector-injector distance is constant for all elements. The main dimensions of the combustion chamber and the injection element are given in Table 1.

The test bench is equipped with various sensors. The chamber pressure is measured at several axial positions. The wall temperature of the combustion chamber is measured for different sensor-wall distances at several axial and azimuthal positions. The temperature and pressure of the coolant water are measured in each water manifold. This way the



Figure 2: Injector Confguration

change in enthalpy of the water can be calculated for each segment and an integral heat load can be derived. A detailed description of the instrumentation is given by Silvestri et al.<sup>20</sup>

So far, tests of the 7-element chamber have been performed for various operating points with combustion chamber pressures ranging from 20 bar to 40 bar and mixture ratios (ROF) of 2.6, 3.0 and  $3.4^{20,22}$  As a reference point for all numerical simulations an operating point of  $p_c = 20$  bar and ROF = 2.6 was chosen.

## 3. Numerical Tools Applied

This section gives an overview on the simulation tools used in the frame of this paper. The main focus is on Rocflam3, which is currently under development and scheduled to replace the current standard heat transfer and performance tool Rocflam-II. The tools used for the simulation of combustion and heat transfer are presented in order of increasing fidelity starting with the 1D system analysis tool RCFS-II in section 3.1. A detailed description of the capabilities of the Rocflam tool family which is capable of both 2D and 3D computations and the new features of Rocflam3 can be found in section 3.2.

A general overview on the current state of methane / oxygen combustion simulation capabilities is given by Riedmann et al.<sup>15</sup> All presented tools have been extensively applied to the combustion simulation of common propellant combinations like hydrogen / oxygen and monomethylhydrazine (MMH) / nitrogentetroxyde (NTO) in the past and results are documented in various publications.

## 3.1 1D - RCFS-II

The heat management is of high importance for the development of any rocket engine thrust chamber. A efficient engineering tool is needed in order to predict heat loads during the design process. At ArianeGroup Ottobrunn, these analyses are done with the in-house tool RCFS-II (Regenerative Coolant Flow Simulation (second generation)). Based on experimental experiences starting in the late 1960s, RCFS-II features Nusselt-type correlations that are anchored on extensive test data for the heat transfer prediction on the hot gas side. Recently, Mäding et al.<sup>8</sup> increased the capabilities of RCFS-II by the implementation of a non-interacting core flow-boundary layer approach that eliminates the need for propellant dependent correction factors. For combustion modeling, equilibrium is assumed and the Gordon-McBride code<sup>10,11</sup> is used for the calculation of the 1D hot gas properties, composition and temperature. The heat conduction through the chamber wall can either be calculated using a 1D plate model approach with fin factor correction or utilizing a 2D FEM structure model. For the heat transfer on the coolant side, Nusselt-type correlations are used and the pressure drop is calculated from 1D analytical models. The above features make RCFS-II the ideal tool for the tailoring of the cooling channel geometry during the thrust chamber design process. Additionally, a loose coupling of RCFS-II for the coolant and structure modeling to higher order CFD solvers for hot gas simulations is possible.

## 3.2 2D & 3D - Rocflam3

Spray combustion tools for rocket combustion chambers have been developed at ArianeGroup Ottobrunn for over 25 years. Rocflam3 is based on that experience and is an evolution of Rocflam-II, which in turn is a merger of the two predecessor codes for storable propellant combinations, ROCFLAM, and for cryogenic applications, CryoROC. It is designated to be ArianeGroups's new standard tool for heat transfer and performance evaluation. Rocflam3 is an in-house developed spray combustion CFD code that solves the Favre averaged Navier-Stokes equations using the SIMPLE algorithm.

Propellant injection can be handled in two ways in Rocflam3. An inlet boundary condition with prescribed mass flow rate can be used which is especially suited for gaseous and supercritical injection conditions. For the injection of liquid propellants the use of a Lagrangian module for droplet tracking and evaporation provides better results. The Lagrangian module is loosely coupled to the Eulerian flow solver. The injected droplets are tracked until vaporization. Mass, momentum and enthalpy transfer to the continuous phase are considered using source terms in the conservation equations. For the current state of the test case both fuel and oxidizer are injected in a gaseous phase, thus the inlet boundary condition was chosen. With the planned transition to liquid injection conditions for the oxidizer the use of the Lagrangian module is envisaged.

Turbulence modeling in Rocflam3 can be done with several two-equation turbulence models. Among others the k- $\varepsilon$ -model of Launder and Sharma,<sup>7</sup> the two-layer-model of Rodi,<sup>16</sup> Wilcox's k- $\omega$  model<sup>24</sup> and the widely spread and well accepted k- $\omega$ -SST model of Menter<sup>12</sup> are implemented. Best results were achieved with the k- $\varepsilon$ -model of Launder and Sharma and the k- $\omega$ -SST model of Menter.

For the modeling of the combustion process one of two different approaches can be chosen. An equilibrium-based pPDF (presumed probability density function) chemistry model is available. The interaction of turbulence and combustion is taken into account by a Gauss- or Beta-PDF. In addition to the governing equations of a non-reacting flow, transport equations for mixture fraction and its variance have to be solved. All necessary fluid and transport properties and the temperature and species composition are tabulated over mixture fraction, mixture fraction variance, enthalpy and pressure beforehand. This equilibrium chemistry model is a good assumption especially for hydrogen / oxygen combustion due to the high reaction rates.



Figure 3: Injection strategy for Rocflam 2D simulations

Table 2: Modified Global Mechanism of Jones and Lindstedt<sup>5</sup>

No	Reaction		
1	CH <sub>4</sub> +0.5 O <sub>2</sub>	$\rightarrow$	$2 H_2 O + 2.24 MJ/kg_{CH_4}$
2	$CH_4+H_2O$	$\rightarrow$	$CO + 3 H_2 - 12.834 MJ/kg_{CH_4}$
3f	$CO + H_2O$	$\rightarrow$	$CO_2 + H_2 + 1.4691 MJ/kg_{CO}$
3b	$CO_2+H_2$	$\rightarrow$	$CO + H_2O - 0.935 MJ/kg_{CO_2}$
4f	$H_2 + 0.5 O_2$	$\rightarrow$	H <sub>2</sub> O+ 119.96 MJ/kg <sub>H<sub>2</sub></sub>
4b	$H_2O$	$\rightarrow$	$H_2 + 0.5 O_2 - 13.423 MJ/kg_{H_2O}$
5f	$O_2$	$\rightarrow$	2 O - 15.574 MJ/kg <sub>O2</sub>
5b	0	$\rightarrow$	$0.5 O_2 + 15.574 MJ/kg_0$
6	$H_2O$	$\rightarrow$	OH + H - 27.708 MJ/kg <sub>H2O</sub>

A second implemented approach is based on a global chemistry with finite reaction rates. Unlike a finite rate chemistry approach that utilizes a full or skeletal reaction mechanism including reactions of short-lived intermediate species, a global chemistry mechanism is reduced to a minimal amount of equations. Reaction rates are either calculated with Magnussen's Eddy Dissipation Concept  $(EDC)^9$  at the fast chemistry limit or the Arrhenius equation. For hydrocarbon fuels like methane, ethanol or kerosene and for the storable propellant combination monomethylhydrazine (MMH) / nitrogentetroxyde (NTO), this chemistry model is better suited. Within this study, a modified Jones-Lindstedt mechanism<sup>5</sup> with modifications according to Frassoldati et al.<sup>4</sup> was used with the implemented reactions of the mechanism shown in Table 2.

For 2D simulations axisymmetry is assumed. Thus, the computational mesh represents only a section of the actual combustion chamber. Instead of resolving the circular element geometry, rings for fuel and oxidizer injection approximate the outer element row as depicted in Figure 3. These rings can either represent the actual element radii or can be tailored for a matching injection surface area. The first approach yields a correct geometric injection position, but leads to a different injection mass flux and momentum whereas the second approach leads to different injection positions but yields the correct injection mass flux and momentum. Experiences with Rocflam-II and Rocflam3 have shown that the first approach is to be preferred.

For 3D calculations a block-structured grid is used. The utilized blocking of a 3D Rocflam3 calculation is shown in

Figure 4(a). Noticeably, the grid doesn't resolve individual injection elements with O-grids. The inlet boundary conditions for oxidizer and fuel respectively are instead mapped to cells which are identified as injection cells as shown in Figure 4(b). Injection cells are defined as cells whose center of area is within the circle defining the injection area.



Figure 4: Grid strategies for Rocflam3 3D computations

## 4. Numerical Setup

This section presents the numerical setup of the different tools. For this paper, all simulations were performed at a reference load point of  $p_c = 20$  bar and ROF = 2.6.

#### 4.1 1D - RCFS-II

To get a first impression of the local heat loads on the hardware, 1D RCFS-II calculations were performed. The hot gas wall contour and cooling channel geometry are described in ASCII-format input files. For the two cooling cycles, mass flow rate, inlet temperature and static pressure are prescribed. Mixture ratio, combustion pressure, combustion efficiency and injection enthalpies of the oxidizer and fuel are defined for the combustion. Hereby, the combustion efficiency is taken from the experimental data.

The results of the RCFS-II simulations are depicted in Figure 5. The resulting wall temperatures at different radial positions are shown in Figure 5(a). As a comparison, measured experimental data at a wall distance of 0.7 mm and 1.5 mm for the first segment (axial coordinates lower than -224 mm) and a wall distance of 1.0 mm for measurement data further downstream is plotted. From these data points the initial wall boundary condition for the 2D and 3D CFD calculation was derived (black dashed line). The red curve represents the wall temperature on the hot gas side whereas the orange curve shows the wall temperature at the bottom of the cooling channel. Both curves show a sharp, discontinuous decrease at the transition from segment 1 to segment 2A and at the transition from segment 3 to the nozzle segment.

The first discontinuity is due to the change in cooling channel geometry. The transition from a rectangular high aspect ratio channel to a cooling channel with circular cross section is linked with a decreased cooling efficiency. This is compensated for by a decreasing wall thickness and a lower total cross sectional area leading to a lowered thermal resistance and an increased Reynolds-number in the cooling channel and thus a higher Nusselt-number respectively. In combination, both phenomena lead to a lower resulting wall temperature. The second sharp decrease in temperature at the transition from segment 3 to the nozzle segment (axial coordinates of -28 mm) can be explained by the change of coolant cycle. The bulk temperature curve depicted in blue shows that the coolant entry temperature of coolant cycle 2 is significantly lower than the exit temperature of coolant cycle 1. Additionally, the coolant mass flow in the nozzle segment is much higher than in the upstream cylindrical segments. This leads to a lower wall temperature despite the generally increased heat flux in the throat region.

As the distance between hot gas wall and coolant channel bottom ranges between 1.0 mm and 1.5 mm, the temperature TWK (orange line) can be compared to the test data. It shows a good agreement for the first segment. In the remaining segments, the measured temperatures of the combustion chamber structure are lower than the simulation results.





(b) Wall heat flux

Figure 5: Results of the RCFS-II simulations

Table 3: Comparison with Experimental Data of Pressure Loss and Heat Pickup for the RCFS-II Simulation

cycle	$\Delta p_{sim}$ [bar]	$\Delta p_{exp}$ [bar]	$\Delta T_{sim}[\mathbf{K}]$	$\Delta T_{exp}[\mathbf{K}]$
1 - cylinder	0.30	1.71	98.8	74.5
2 - nozzle	1.31	10.84	5.9	4.0

The observed steep gradients in the simulated temperature profiles would not occur in reality due to axial heat conduction. This phenomenon is not considered by RCFS-II and a 3D structure model would be needed to correctly predict its influence. The missing axial heat conduction might also explain the slightly higher temperatures in the simulation. As the nozzle segment is cooled significantly more than the cylindrical section of the combustion chamber, its structure serves as a heat sink and thus lowers the temperature of the upstream segment 3. As RCFS-II is a 1D tool based on an equilibrium approach, the wall pressure loss in the cylindrical section of the combustion chamber can only be approximated. For the performed simulations we forwent this option and chose a constant wall pressure instead.

The simulated heat flux profile is shown in Figure 5(b). The red curve shows the local wall heat flux. From the experiment only a segment averaged wall heat flux can be obtained. This heat flux is represented by the green curve. For better comparison to the test data, the simulation results are averaged by segment as represented by the orange curve. The averaged heat flux agrees very well with the experimental data. Only for the segments with drilled cooling channels (2A, 2B and 3), the simulated heat flux is higher than the measured one. This can also be attributed to the overprediction of the cooling efficiency in those segments.

A comparison of numerical and experimental data for the pressure loss and temperature increase of the coolant by coolant cycle is given in Table 3. The pressure loss for the first coolant cycle (i.e. the cylindrical section) matches very well. The predicted pressure loss is slightly lower than the one obtained in the experiments due to the neglection of losses in the water transition manifolds between segments. The temperature increase of the coolant water in the cooling channels is predicted to be higher than the measurements. This is due to the aforementioned overprediction of the heat flux in the segments with circular cooling channel cross sections.

For the second coolant cycle (i.e. the nozzle segment), the temperature increase of the coolant is predicted very well. The pressure loss however is predicted to be much lower. Analytic calculations show again that the main portion of the pressure loss is due to the inlet and outlet manifold. These losses are not considered as the RCFS-II model only contains the cooling channels.

## 4.2 2D - Rocflam3

Before the execution of computationally expensive 3D Rocflam3 calculations an extensive parameter study on a 2D grid was performed. The 2D simulations allow for a quick parameter variation and the characterization of the influence of the computational grid and various modeling parameters.

As inlet boundary conditions for oxidizer and fuel, the mass flow and inlet temperature from the experiment are



Figure 6: Computational grid for 2D Rocflam3 calculations (vertical dimension magnified by factor 10)



Figure 7: Dimensionless wall distance  $y^+$  of the chosen computational grid

taken. The faceplate is assumed to be adiabatic. For initial simulations the hot gas wall temperature is derived from the experimental data. The global chemistry approach presented in section 3.2 with the modified Jones-Lindstedt mechanism is used as combustion model.

In order to reach mesh convergence, an extensive mesh study was performed. The axial mesh resolution near the faceplate, in the cylindrical part of the chamber and in the throat region together with the radial resolution in the core flow and boundary layer region were varied independently in over 50 combinations. The resulting mesh has 66 560 finite volumes and is depicted in Figure 6. The dimensionless wall distance  $y^+$  of the wall nearest cell is in the order of 1 for all calculations as shown in the exemplary plot in Figure 7.

Second order accuracy for the numerical flux computation is ensured by using the SUPERBEE<sup>17</sup> scheme. For all performed simulations the SST turbulence model was chosen. Heat transfer and combustion efficiency are influenced by the model parameters of the turbulence model. Those parameters, the turbulent Prandtl- and the Schmidt-number, have to be set by comparing the simulation results to the test data. The turbulent Prandtl number

$$Pr_t = \frac{\mu_t c_p}{\lambda_t} \tag{1}$$

represents the ratio of turbulent momentum and heat transport and normally ranges between 0.5 and 1.0. It has a major impact on the wall heat flux. The turbulent Schmidt number

1

$$Sc_t = \frac{\mu_t}{\rho D_t} \tag{2}$$

is the ratio of turbulent momentum and mass transfer and directly influences the mixing in the combustion chamber. It normally ranges between 0.7 and 1.0. Both parameters are set constant over the entire domain. Unlike many commercial codes like e.g. CFX, Rocflam3 allows the independent variation of turbulent Prandtl- and Schmidt-number, i.e. a turbulent Lewis-number  $Le_t = Sc_t/Pr_t$  not equal to unity. A comparison of the computed wall heat flux and normalized wall pressure profiles to the test data is given in Figure 8(a) and Figure 8(b). The heat flux is area averaged for every calorimetric segment. The wall pressure is normalized by the last axial pressure signal. As can be seen in Figure 8(b), the wall pressure profile of the simulation with a turbulent Schmidt number of 0.8 and a turbulent Prandtl number of 0.8 agrees very well with the experimental data. The wall heat flux shows good agreement for a setting of  $Sc_t = 0.9$ and  $Pr_t = 0.9$  up until the nozzle segment where none of the performed simulations give satisfactory results.

As Rocflam3 does neither resolve the injection element nor the shear layer explicitly, the turbulence intensity at the inlet boundary condition can heavily influence the resulting flow field. For the chosen grid and a compromised setting of  $Sc_t = 0.8$  and  $Pr_t = 0.9$ , a variation of the turbulence intensity at the inlet was performed. The respective simulations did not converge for turbulence intensities lower than 0.15. The necessity of a high turbulence intensity at the inlet is due to the rather coarse mesh resolution in the mixing zone close to the injectors.

The results for turbulence intensities ranging from 0.15 to 0.3 are shown in Figure 9(a) and Figure 9(b). The data in Figure 9 shows a minor influence on wall heat flux and wall pressure. In general, a higher turbulence intensity leads to better mixing and therefore a faster combustion process. This can be noted by the slightly increased wall heat flux for the first two segments with increasing turbulence intensity. As noticed before, the heat flux prediction in the last two segments is not as good as in the first segments. Here, the turbulence intensity has a negligible influence. The



(a) Segment averaged wall heat flux

(b) Wall pressure normalized with last measured pressure

Figure 8: Prandtl and Schmidt number variation for Rocflam3



(a) Segment averaged wall heat flux for  $Sc_t = 0.8$  and  $Pr_t = 0.9$  and varying turbulent intensity at the inlet



Tu = 0.15 Tu = 0.2

Tu = 0.3

experiment

(b) Wall pressure normalized with last measured pressure for  $S c_t = 0.8$  and  $Pr_t = 0.9$  and varying turbulent intensity at the inlet

Figure 9: Inflow turbulent intensity variation for Rocflam3

setting of Tu = 0.2 shows good agreement with the test data for both wall pressure and heat flux and thus is used for all following simulations.

For the final setting of  $Sc_t = 0.8$ ,  $Pr_t = 0.9$  and Tu = 0.2, a detailed examination of the numerical results is performed. These are given in Figure 10 with the resulting temperature and mixture ratio fields shown in Figure 10(a), the wall heat flux shown in Figure 10(b) and the resulting normalized wall pressure shown in Figure 10(c). For both the wall heat flux and wall pressure, experimental results are added to the plots as comparison.



(a) Temperature and oxidizer to fuel ratio for  $Sc_t = 0.8$ ,  $Pr_t = 0.9$  and Tu = 0.2 (vertical axis scaled by 2)



Figure 10: Simulation results of the Rocflam3 2D calculations with  $Sc_t = 0.8$ ,  $Pr_t = 0.9$  and Tu = 0.2

Figure 10(a) shows the temperature field on the upper half and the local oxygen to fuel mixture ratio on the lower half. The stoichiometric mixture ratio  $\text{ROF}_{st} = 4.0$  is denoted by the black line. Both the temperature and the mixture ratio plot show a significant difference in flame length between the outer element row and the central element. The elongation of the stoichiometric zone which can be interpreted as the reaction zone is much shorter on the axis than for the outer row. The injected oxygen travels nearly halfway downstream the chamber as opposed to the short GOX kernel for the central element. In Figure 10(c), it can be seen that the pressure prediction of Rocflam3 is very good. However, the wall heat flux is underpredicted in the last segment as indicated in Figure 10(b).

As the application of the global chemistry model underestimates the wall heat flux in the convergent-divergent nozzle, a cross-check with the equilibrium chemistry model was conducted. The grid and the model parameters of the turbulence model as well as the boundary conditions were kept constant.

A first comparison of the temperature field for the global chemistry and the equilibrium chemistry model visualized in Figure 11 shows that both models yield qualitatively rather similar results. The global chemistry approach predicts generally higher combustion temperatures in the shear layer near the injection elements. The stoichiometric zone, indicated by the black line in both figures, shows a slightly longer flame on the axis for the global chemistry and a closed combustion zone for the elements on the outer row. In contrast, using the equilibrium chemistry leads to an



#### global chemistry

Figure 11: Comparison of the temperature field for the global chemistry and the equilibrium chemistry modeling approach (vertical axis scaled by 2)



(a) Comparison of the wall heat flux for the global chemistry (solid) and the equilibrium chemistry (dashed) modeling approach



(b) Comparison of the normalized wall pressure for the global chemistry (solid) and the equilibrium chemistry (dashed) modeling approach

Figure 12: Comparison of the normalized wall pressure for the global chemistry (solid) and the equilibrium chemistry (dashed) modeling approach

open stoichiometry zone indicating a not fully completed combustion. This elongated reaction zone of the equilibrium model can be attributed to insufficient mixing.

The normalized wall pressure profiles for both chemistry models are depicted in Figure 12(b). Noticeably, the equilibrium chemistry model leads to a lower pressure than the global chemistry approach. This can be correlated to the unfinished combustion process in this case as indicated by the open stoichiometric zone in Figure 11 for the outer injection element. A closer look on the local and segment wise averaged wall heat flux in Figure 12(a) reveals that the global chemistry model predicts good results for the cylindrical sections while the equilibrium model yields better results regarding the maximum wall heat flux in the throat section. The increased heat flux of the equilibrium model in the segments 2A, 2B and 3 also explains the lower temperatures observed in Figure 11 as more energy is extracted towards the defined wall boundary condition.

## 4.3 3D - Rocflam3

3D simulations were performed with Rocflam3 to conduct a detailed analysis of the 7-element combustion chamber. The combustion chamber shows a rotational symmetry for  $30^{\circ}$  segments. In order to fully resolve an injection element on the outer row, a  $60^{\circ}$  segment was chosen as computational domain.

The axial and radial resolutions are set to be identical to the 2D grid as an outcome of the extensive 2D mesh study. A variation of the azimuthal resolution was performed until mesh convergence was observed. The resulting mesh has 5 317 600 cells.

Employing the same methodology, the setup resulting from the detailed 2D evaluation on the influence of the turbulent Prandtl- and Schmidt-number as well as the turbulence intensity at the inlet is adapted for the 3D case. The results of the 3D simulation with a setting of  $Sc_t = 0.8$ ,  $Pr_t = 0.9$  and Tu = 0.2 are shown in Figure 13, Figure 14 and Figure 15.



Figure 13: Temperature for  $Sc_t = 0.8$ ,  $Pr_t = 0.9$  and Tu = 0.2

Figure 13 shows the temperature in the flow field at various axial slices and the stoichiometric iso-surface. The stoichiometric surface can be interpreted as the main reaction zone and indicates the flame position. Noticeably, the flame of the element on the outer row extends further downstream than the flame on the chamber axis.

The local wall heat flux is depicted in a top view in Figure 14. It can be seen in the figure that the maximum heat flux occurs in the throat at the azimuthal position of the outer injection element. A second area of increased wall heat flux prior to the throat can also be recognized. This region can be interpreted as the zone in which the flame approaches the combustion chamber wall.

Temperature and mixture ratio are visualized in sections along the chamber axis in Figure 15. The upper image, Figure 15(a), shows a cut through the center of both the outer and the central injection element. The difference in flame length and GOX kernel length between the central and outer injection element can be seen. In the lower image, Figure 15(b), a cut through the central element and the position between two elements on the outer row is depicted. The stoichiometric mixture ratio is denoted by the black line to visualize the flame position.

In Figure 16 the axial profiles of the wall heat flux and the normalized wall pressure are compared to the available test data. On the left in Figure 16(a), the azimuthal variation of the heat flux is depicted by the blue dotted lines. The continuous blue lines give the minimum and maximum azimuthal heat flux correlating with the position between two outer injection elements and the element center position, respectively. The pink line indicates the azimuthal mean heat flux curve. The segment wise averaged heat flux is shown in red for comparison to the test data (green). Especially within the throat segment, the calorimetric heatflux is underestimated by the numerical solution. On the right in Figure 16(b), the normalized wall pressure is provided together with the experimental data. Hereby, the last measurement point is used for normalization. The comparison shows that the 3D simulation using Rocflam3 predicts lower pressure values.

## 5. Discussion

### 5.1 Influence of chemistry modeling

As already discussed in section 4.2 neither of the two chemistry models provide a good prediction of the wall heat flux for both the cylindrical section of the combustion chamber and the throat region. The global chemistry approach leads



Figure 14: Local wall heat flux in top view on combustion chamber wall (vertical axis scaled by 2)

T [K]: 300 1300 2300 3300	
ROF: 0 2 4 6 8 10	
(a) Temperature and ROF at outer injector plane T [K]: 300 1300 2300 3300	

ROF: 0 2 4 6 8 10

(b) Temperature and ROF between outer injector positions

Figure 15: Simulation results of the Rocflam3 3D calculations with  $Sc_t = 0.8$ ,  $Pr_t = 0.9$  and Tu = 0.2 (vertical axis scaled by 2)

to a good prediction for the first four segments (1, 2A, 2B, 3), but predicts a low heat flux for the throat region whereas the equilibrium model matches the heat flux in the throat region rather well but overpredicts the heat flux intensity for segments 2A, 2B and 3. This general behavior has also been observed in 3D simulations. Both models have in common a rather small increase of the segment averaged heat flux from segment 3 to the nozzle segment.

In general, the equilibrium model leads to lower pressures than the global chemistry approach. This has been attributed to a insufficient mixing in case of the equilibrium model. This may be an indicator that a different setting of the turbulence model parameters has to be chosen for the equilibrium model compared to the global chemistry model in order to increase mixing and lower the heat transfer intensity.

## 5.2 Tool comparison

In Figure 17, the wall heat flux q is shown including the 1D RCFS-II results together with the numerical data obtained within 2D and 3D Rocflam3 simulations. Hereby, the continuous lines represent the calorimetric q and the dashed lines the respective local q. Considering the first four segments encompassing the cylindrical part, the predicted heat flux



(a) Wall heat flux

(b) Normalized wall pressure

Figure 16: Comparison of the results of the 3D simulation to the experimental data

of the 3D simulation using Rocflam3 best matches the experimental data. Both the 1D and 2D approaches give higher values of q for the central segments 2A, 2B and 3. In the converging-diverging throat section, RCFS-II agrees best with the measured values while both Rocflam3 solutions underestimate the calorimetric heat flux by 4 to 5 MW/m<sup>2</sup> respectively. These differences might be attributed to a unphysical temperature boundary condition provided at the hot gas wall, which has been set constant using the last measured temperature in the upstream cylindrical section. For a more accurate wall heat flux prediction using Rocflam3, a coupled simulation incorporating the coolant flow would be required. The potential improvement is indicated by the RCFS-II solution using a 1D coupling.

For the 2D and 3D simulations using Rocflam3, the temperature distribution is visualized together with a line for the stoichiometric mixture ratio in Figure 18. Both approaches correlate by predicting a longer flame for the outer injection element. However, a smaller difference between the two flames can be observed for the 3D simulation. Compared to the 2D results, the outer flame length is reduced. This might be due to the correct representation of the momentum ratios using a 3D flow configuration leading to an enhancement of the diffusive mixing and therefore an acceleration of the chemical reaction. The reduced stratification in the temperature distribution confirms this enhanced mixing process for the 3D simulation as downstream of the stoiciometric mixture ratio, the 2D computation predicts relatively cold core temperatures near the center axis of the combustion chamber. Another difference can be observed in the shear layer region following the faceplate, for which the 2D simulation predicts higher temperatures. This effect might be attributed to the faster flow acceleration after injection observed within the 3D results, possibly due to the enhanced momentum exchange. The resulting faster downstream transport of the mixture delays the formation of high temperature regions.

## 6. Outlook

The discussion in section 5 led to the conclusion that neither chemistry model in Rocflam3 correctly predicts both wall heat flux and wall pressure. One way to overcome this problem is the introduction of a new chemistry model. As a full finite rate chemistry is not feasible in an industrial frame, the flamelet model first described by Peters<sup>13</sup> could possibly lead to improvements in the predictive capabilities of Rocflam3. Efforts are currently underway to implement the flamelet model with a future augmentation to allow for a non-adiabatic wall treatment being envisaged.

In the context of the SFB-TRR 40 summer program 2017 a comparison of the achieved simulation results with several other academic groups utilizing various CFD codes will be performed. In the same project, the maturation of Rocflam3 towards an efficient 3D simulation for full scale thrust chambers is promoted.

In order to better transfer the obtained data to full scale rocket combustion chamber applications which usually involve the injection of liquid oxygen, the experimental setup is currently modified for the use of LOX as oxidizer in the frame of a project sponsored by BFS. First experiments at TUM are expected for 2018.



Figure 17: Comparison of the segment averaged wall heat flux for the applied tools (dashed line: mean heat flux)



Rocflam3 2D

Figure 18: Simulation results of the Rocflam3 2D and 3D calculations with  $Sc_t = 0.8$ ,  $Pr_t = 0.9$  and Tu = 0.2 showing the temperature distribution and stoiciometric mixture ratio (vertical axis scaled by 2)

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