Comparison of different modeling approaches for CFD simulations of a single-element GCH₄/GOX rocket combustor

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As part of the Combustion Modeling Workshop during the SFB/TRR 40 Summer Program 2015 at the Technische Universität München, numerical simulations of flow and combustion in a single-element GCH₄/GOX rocket combustor have been performed using different modeling approaches implemented in different computational tools. The differences and commonalities between these approaches and tools are outlined in this report. The results obtained with the different tools for a common operating point are presented. They show large discrepancies in the prediction of relevant validation and design parameters. The causes for these discrepancies are discussed. In addition the numerical results are compared to the experimental data obtained at the Institute for Flight Propulsion at the Technische Universität München for the simulated operating point.

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1. Introduction

Numerical simulations of flow and combustion in liquid rocket engine thrust chambers can be used to support the layout and optimization of new component designs and reduce the development time and cost [1]. The numerical tools used must be able to accurately predict relevant design parameters, such as heat load on the chamber wall, combustion pressure and combustion efficiency as well as performance parameters. In order for a tool to be reliably used in the design process, it must encompass numerical models that describe the physical processes in a rocket engine accurately enough to make design choices without being prohibitive to use with regard to computational time. Furthermore, these models must be applicable and validated for the wide range of operating conditions which can occur in different types of rocket engines (e.g. launcher propulsion, attitude control thrusters).

In order to help with the validation of numerical tools focussing on rocket engine design, the Institute for Flight Propulsion at the Technische Universität München has tested

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several different configurations of rocket combustors and propellant combinations, building an experimental data base which can be used in the validation process. As part of the SFB/TRR 40 Summer Program 2015 a test case from this data base was defined. The description of the complete test case can be found in [2] including all the relevant boundary conditions and is summarized in Sec. 2.

In the present paper the results for the prediction of relevant design parameters employing different models and numerical tools are presented in a comparative manner. The simulations were performed by different research groups as part of the SFB/TRR 40 Summer Program 2015. The paper summarizes the major differences between the different tools and lists the models used for the simulation of the test case. All simulations were performed without a priori knowledge of the experimental results to facilitate a 'blind test'.

This paper is structured as follows. First the reference experiment conducted at the Institute for Flight Propulsion is introduced in Sec. 2. In Sec. 3 the different numerical setups are described briefly and the results obtained are compared against each other and against the experimental data. Section 4 summarizes the simulation results on an individual bases and gives more insight into the respective tools used and a conclusion on the results obtained. Section 5 then gives an overall conclusion on the results obtained and the necessary steps for improvements.

2. Test case

In [2] a test case for the validation of CFD tools concerned with the modeling of flow and combustion in rocket thrust chambers is presented. The experimental setup features a combustion chamber with a square inner cross section and a single coaxial-type injection element, that is flush mounted to the faceplate. At the end of the chamber the combustion gases are expanded to ambient pressure in a convergent-divergent nozzle with a rectangular throat area. A CAD model of the combustor operated at the Institute for Flight Propulsion at the Technische Universität München is shown in Fig. 1. The contraction ratio in the tested configuration is 2.5, which is close to typical values that can be found in actual flight hardware (Vulcain: 2.5, Aestus: 2.38, HM7: 2.78). This is unlike other test cases that have been proposed in past rocket combustion modeling workshops [3], [4]. The chamber is operated with gaseous methane as fuel and gaseous oxygen as oxidizer. The presented nominal operating point is at an oxidizer to fuel ratio of 2.6 and a combustion pressure of 20 bar. The mass flow to the combustion chamber is set using sonic orifices in the feed line.

The combustion chamber and the nozzle are made of oxygen-free copper and the whole assembly is capacitively cooled. Due to the nature of the cooling the chamber is only operated for a limited amount of time per hot firing test and therefore the nature of the test case is transient. In a typical test firing the combustor is operated for 3 s. The combustion pressure is measured by multiple pressure transducers distributed in axial direction along the inner chamber wall. The temperature in the chamber wall is measured by multiple clusters of thermocouples located in the chamber material itself, in short distances from the hot gas wall side. The measured temperature profile averaged over 0.5 s at 2/3 of the burning time is used to reconstruct the hot gas wall temperature as a boundary condition for numerical simulations and to calculate the heat flux to the chamber wall as a parameter for the validation. The combustion efficiency is calculated using the procedure outlined in [5]. The values of the experimental data used for the
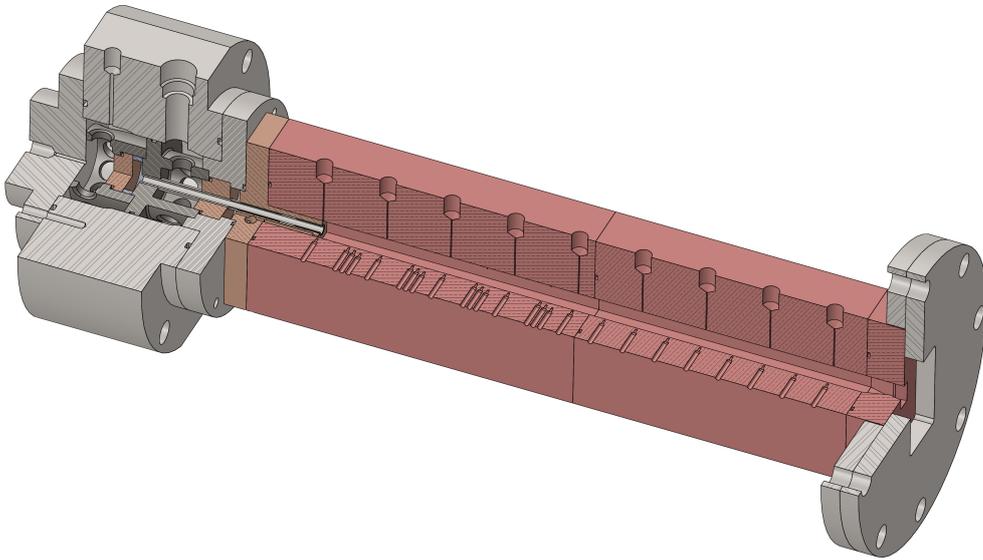
FIGURE 1. CAD model of the tested single-element rocket combustor.

tool validation are not included in the test case description [2], but were given to the workshop participants for comparison after preliminary results with the different tools were achieved. This was done to facilitate the idea of a predictive simulation in a 'blind test'.

3. Comparison of different modeling approaches

During the SFB/TRR 40 Summer Program 2015, eight different simulation results for the test case described in Sec. 2 were presented. The results were achieved by seven individual research groups employing different physical models and numerical tools. Airbus DS presented two results from two different tools. The participating groups and a general overview of their employed models and computational setup is given in Tab. 1. In this section the results are discussed in a comparative manner. The next section features the discussion of the individual results.

Out of the eight simulations performed during the workshop, six are RANS simulations, while only one URANS (UniBW) and one LES (CERFACS) simulation was performed, respectively. The grid resolution varies drastically from 50 million cells for the LES simulation to only 45 thousand cells for the simulation of the test case on a coarse common grid that was agreed on during the workshop. However, only three groups presented their results for the coarse common grid here, namely Airbus DS (Rocflam3), UniBW and TUM-LFA. The TUM-TD group presented their results for a medium fine common grid. The results of the other groups shown here are the ones achieved with their individually chosen setup that represented their most confident result. The JAXA group as well as the group from the IVLR performed 3D simulations of a quarter of the chamber, while most other groups performed 2D axisymmetrical simulations of the configuration. Only the CERFACS group presented a full 3D simulation. All groups except CERFACS used classical RANS turbulence models and a fully resolved wall treatment.

Groups	Airbus DS	Airbus DS	CERFACS	JAXA	TUM-LFA	TUM-TD	UniBW	IVLR
Code	CFX	Rocflam3	AVBP	CRUNCH-CFD	FLUENT	FLUENT	OpenFoam	TASCOM3D
Equations	RANS	RANS	LES	RANS	RANS	RANS	URANS	RANS
2D/3D	2D	2D	3D/full	3D/quarter	2D	2D	2D	3D/quarter
Solver	pressure based coupled	pressure based SIMPLE	density based TTGC	density based SIMPLE	pressure based coupled	pressure based PISO	pressure based	density based
Grid cells	$51 \cdot 10^3$	$45 \cdot 10^3$	$50 \cdot 10^6$	$3 \cdot 10^6$	$45 \cdot 10^3$	$175 \cdot 10^3$	$45 \cdot 10^3$	$835 \cdot 10^3$
Post tip cells	6	5	20	15	5	10	5	32
Turbulence Models	k-ω SST	k-ϵ low-Re	Smagorinsky wall-functions	k-ϵ two-layer	k-ϵ two-layer	k-ω SST	k-ϵ low-Re	k-ω SST
Combustion Models	Flamelet	Eddy dissipation & Arrhenius	Finite rate	Finite Rate	Equilibrium	Flamelet	Flamelet	Finite Rate
TCI	Beta-PDF	laminar	resolved	laminar	Beta-PDF	Beta-PDF	Beta-PDF	laminar
Chemistry	ANSYS C1	7 species 3 reactions	13 species 73 reactions	21 species 97 reactions	11 species	21 species 97 reactions	GRI 3.0	21 species 97 reactions
Prt/Sct	0.9/0.9	0.85/0.85	0.6/0.6	0.9/0.9	0.85/0.85	0.85/0.85	0.85/0.85	0.7/0.7
Injector Resolved	no	no	yes	yes	no	no	no	yes

TABLE 1. Overview of employed physical models and computational setups.
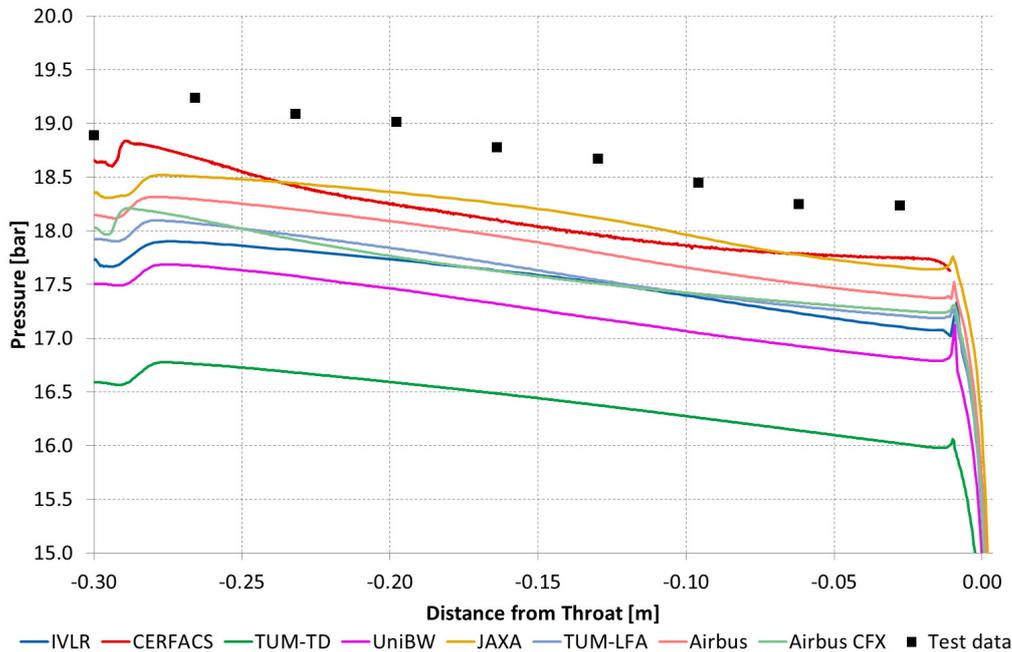
FIGURE 2. Axial profiles of absolute pressure.

The CERFACS group chose to use a wall function modelling approach for their LES instead. A great variety of combustion models was used. Details are described in the discussion of the individual results. Notably three groups, JAXA, TUM-TD and IVLR used a chemical kinetic scheme, that was specifically developed for this application as part of the SFB/TRR 40 program [6].

   The main validation data gained from the experiment are the wall pressure profile and the wall heat flux in axial direction, which has been reconstructed from thermocouple measurements inside the chamber wall as described in [7]. In the following the results for these validation parameter from the simulations are compared against each other and against the experimental data.

   Figure 2 shows the absolute pressure profile in axial direction along the combustion chamber wall for all performed simulations. It also includes the measurements from the pressure transducers acquired during the hot firing test. As can be seen in the graph, all simulations underpredict the experimental wall pressure considerably. In general the chamber pressure in a rocket combustor for a given mass flow rate and throat area is determined by a balance between the heat released by the combustion and the heat loss to the chamber wall. Therefore, the underprediction of the absolute chamber pressure is most likely connected to either an underpredicted combustion efficiency, due to a mixing or reaction progress problem, or an overprediction of the wall heat flux by the simulation.

   In Fig. 3 the normalized pressure profiles are presented. As normalization factor the pressure at the last measurement point was chosen, so that all curves intersect in that point. As the shape of the pressure profile is linked to the heat release rate, conclusions about the combustion progress can be drawn from these profiles. None of the simulations predict the steep rise between the first two measurement points and only the LES simulation performed by the CERFACS group captures the low gradient between the
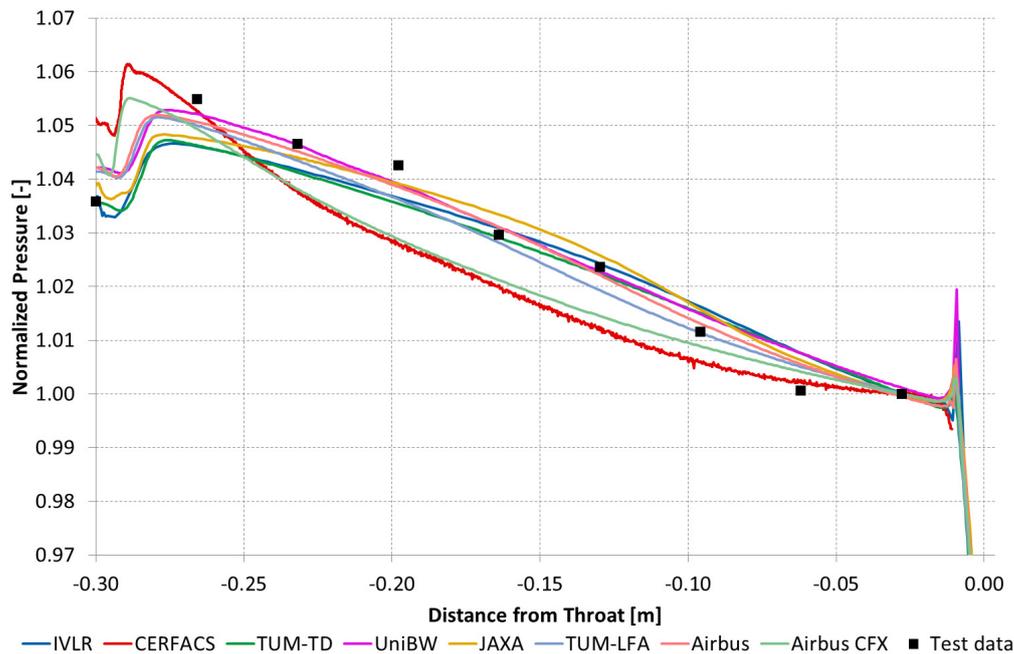
FIGURE 3. Axial profiles of normalized pressure.

last two measurement points. The CERFACS simulation and the Airbus CFX simulation predict a stronger, earlier heat release and therefore a steeper pressure gradient in the first part of the chamber. Both these simulations notably show a concave pressure profile while all the other simulations and the experimental data seem to suggest a convex one. The test data also seems to indicate that the combustion process is finished before the convergent part of the nozzle, while most simulations predict the opposite. The simulations that predict the flat profile at the end of the combustor do not match the measurements in the beginning very well, due to a high heat release rate, which in turn explains the flattening of the profile in the end.

For the type of CFD simulation performed in this study an accurate prediction of the wall heat flux in the combustion chamber is critical. The heat flux is not only a validation parameter which can be gained from hot firing tests, it is also a critical design parameter used for structural analysis and cooling layout during the design phase. Figure 4 shows the wall heat flux along the top wall of the combustion chamber from all simulations and the values reconstructed from the thermocouple measurements during the test. Most simulations do not capture the steep rise in the beginning of the combustion chamber and overestimate the flux throughout most of the chamber. A wide spreading of the prediction of the heat flux peak in the throat can be seen in the results. This is critical, as the throat is generally the part that experiences the strongest heat load. The predictions range from the lowest heat flux of about 6 MW/m^2 by the TUM-TD group to the highest of 21 MW/m^2 by JAXA. The simulations also differ strongly in the predicted heat flux rise in the nozzle compared to the highest value found in the chamber before the convergent part.

In Fig. 5 the temperature field predicted by the simulations is shown. As can be seen in the temperature fields, the simulations differ in the prediction of the flame length and the
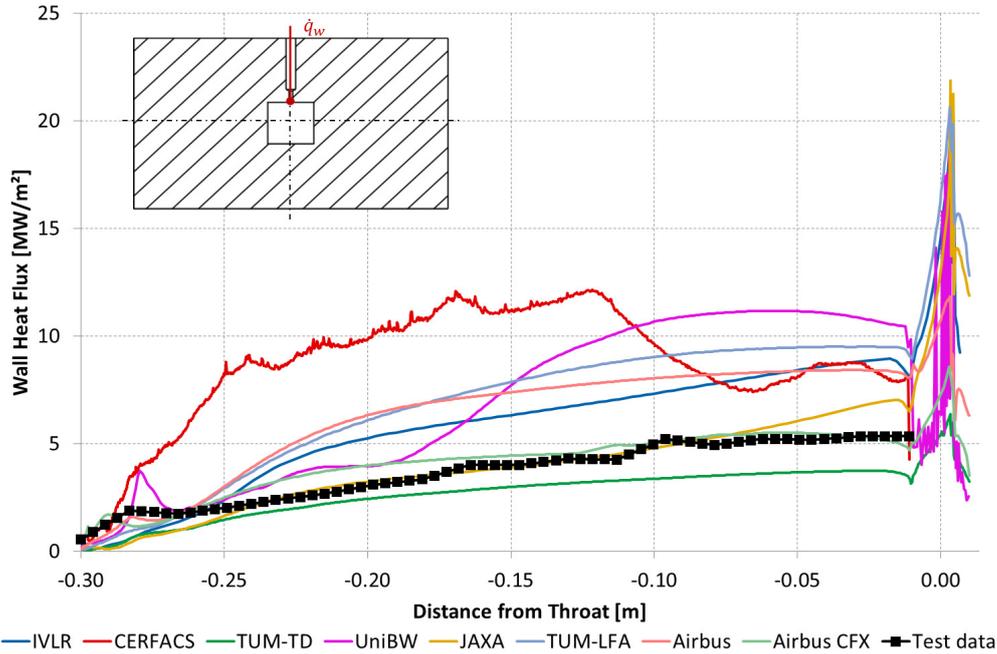
FIGURE 4. Wall heat flux along the upper wall of the combustion chamber.

prediction of the maximum temperature. The predicted values for the maximum temperature are given in Tab. 2. The calculated equilibrium temperature at the stoichiometric mixture fraction and a combustion pressure of 19 bar is 3443 K in the adiabatic case and can be regarded as the maximum theoretically possible temperature. Depending on the combustion model and the chemical kinetic scheme used, the different simulations are closer or further away from this maximum temperature. The models using finite rate chemistry, see Tab. 1, get close to this temperature, while models using a PDF approach for turbulence chemistry interaction show lower temperatures. The simulation performed by Airbus DS with Rocflam3 and a global reaction scheme notably exceeds the equilibrium temperature.

Table 2 also includes the length of the recirculation zone. Most simulations predict it to be between 17 and 22 mm in length. Only the CERFACS and the Airbus DS CFX simulation predict it to be shorter with 10 mm and 14 mm respectively. The prediction of the recirculation length is important in this test case as it is related to the prediction of the pressure and heat flux peak in the near injector region.

4. Discussion of individual results

4.1. *Technische Universität München, Institute for Flight Propulsion (LFA)*

The simulation results presented here are 2D axisymmetric and were performed on a coarse common grid that was agreed upon by the participating groups during the SFB/TRR 40 Summer Program 2015. However, only the Airbus DS Rocflam3, the UniBW and the TUM-LFA groups presented their results for this grid. The grid is the coarsest one used in this report with approximately 45 thousand cells.

The Institute for Flight Propulsion at the Technische Universität München is working
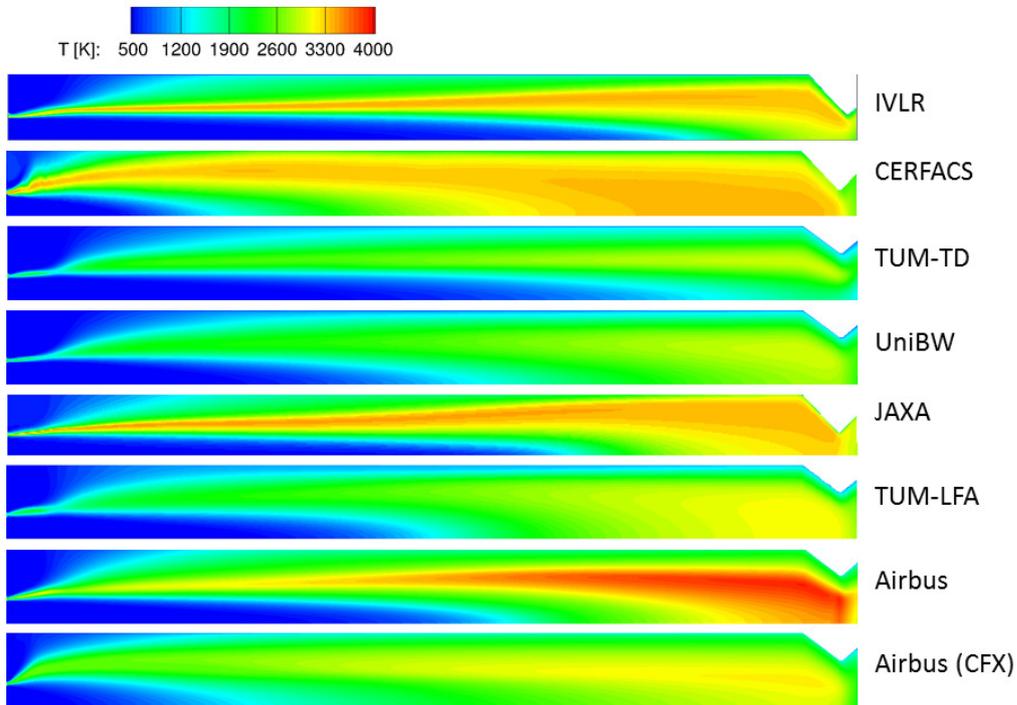
FIGURE 5. Temperature field inside the combustor.

Groups	Airbus CFX	Airbus Rocflam3	CERFACS	JAXA	TUM-LFA	TUM-TD	UniBW	IVLR
Maximum Temperature in K	3366	3943	3464	3446	3160	2956	2966	3425
Recirculation in mm	10	18	14	17	20	19	20	17

TABLE 2. Comparison of distinct values.

on adapting the commercial CFD code ANSYS Fluent for use in rocket engine design and analysis. The models used are summarized in Tab. 1. The standard k-ϵ model with enhanced wall treatment was chosen as turbulence model. This model allows resolving the wall with a dimensional wall distance lower than one, employing a two-layer approach.

The combustion was modeled using tabulated chemistry employing an equilibrium assumption. The table is generated using a non-stoichiometric algorithm based on Gibb's free energy minimization. With this approach the presented setup is the only one out of the participating groups that does not require a chemical kinetic mechanism.

The normalized pressure profile, see Fig. 5, compares well with the other codes and also the experimental data. Only the steep rise at the first two measurement points is

not reflected very well. Also the plateauing effect that seems to be indicated by the experimental data is not captured. The absolute pressure is predicted about 1 bar to low.

The wall heat flux shown in Fig. 4 is overestimated considerably by the simulation compared to the test data. This has a direct effect on the combustion pressure which could explain the too low value at least partly. There is however also a question about the correct prediction of the mixing process, which, if predicted to be to low, leads to an underestimation of the total heat released by the combustion.

An open issue is the choice of the turbulent Prandtl and Schmidt number. In this setup the Fluent defaults of 0.85 have been used. The appropriate choice of these values is a critical point at the LFA going forward as they have a significant impact on the prediction of the validation parameter.

Another point of further investigation will be to clarify whether the approximation of chemical equilibrium is justified for methane/oxygen combustion.

Furthermore, a 3D model of the combustion chamber is going to be investigated. The purpose of this is to quantify the influence of the corner effects produced by the rectangular cross section of the inner combustion chamber. The 2D simulations were helpful for first quick turnaround simulations and the code comparison but their accuracy for a chamber with 3D effects still has to be investigated.

4.2. *Airbus DS (Rocflam3)*

The Airbus DS Rocflam3 simulations that are discussed here are performed in a 2D axisymmetric domain on a grid which has been set up by the participating groups together in order to enable a better comparison between the RANS results. In the end, only TUM-LFA, UniBW and Airbus DS have shown solutions obtained on this common grid at the final presentation of the summer program. Therefore, the TUM-LFA and UniBW simulations are performed on the same grid. This common grid is the coarsest one that is considered in this tool comparison. TUM-TD uses a refined version of the common grid. As documented in Tab. 1, the low-Re k-ϵ model by Launder & Sharma [8] is used for turbulence modeling and a mixed finite rate/EDC approach is used for combustion modeling (EDC: Eddy Dissipation Concept, see Magnussen & Hjertager [9]). A global reaction mechanism with seven species and three reactions based on the scheme by Westbrook & Dryer [10] is tested here. Table 1 shows that this is by far the smallest mechanism used within this tool comparison.

Regarding the normalized pressure profile shown in Fig. 3 Rocflam3 compares well with the other codes but neither captures the steep rise between the first two data points nor the low gradient between the last two data points. The absolute pressure profile (see Fig. 2) shows that Rocflam3 computes a comparatively high pressure level which is however still about 1 bar below the measured one.

In comparison with the available test data for the specific wall heat flux shown in Fig. 4, it can be seen that Rocflam3 overestimates the test data significantly downstream of about -0.27 m. The resulting overestimation of the deducted heat is in line with the underestimation of the chamber pressure. However, as visualized in the temperature contour plot in Fig. 5, the temperature level is extremely high in the Rocflam3 result: The maximum value lies around 4000 K, while the equilibrium value for an ideal rocket is 3443 K. This significant overestimation of the hot gas temperature for sure has an influence on the wall heat flux and is almost certainly a defect of the small chemistry mechanism which is applied here. Therefore, the combustion and chemistry modelling approach will be revised in the near future. This is considered to be the most important

step for Rocflam3 in order to achieve better results for this test case.

Another important aspect of the available simulation results is the maximum wall heat flux in the throat region. The Rocflam3 value belongs to the lower ones of the present comparison. Another Rocflam3 simulation with a 2-layer turbulence model by Chen & Patel [11] and apart from that unchanged settings shows a 38 % higher maximum heat flux while the level in the cylindrical part remains almost the same. According to our experience with both turbulence models, this is not generally the case for the simulation of thrust chambers with Rocflam3 using these turbulence models. Nevertheless, the choice of the turbulence model must also be revised. Unfortunately, the present test case does not offer experimental data in the throat region.

The last point to be discussed here is the choice of the turbulent Prandtl and Schmidt numbers. Considering only the RANS and URANS simulations in this comparison, the choice varies between $Pr_t=Sc_t=0.7$ and $Pr_t=Sc_t=0.9$. As has been shown in the outline presentation, the influence of these parameters is significant. Therefore, it is desirable that everybody has a similar understanding of how to choose them and that everybody knows how important it is to discuss them.

4.3. *Airbus DS (CFX)*

The Airbus DS CFX simulations that are discussed here are performed in a 2D axisysmmetric domain on a rather coarse mesh with $50 \cdot 10^3$ grid cells. The well-known SST model is applied for turbulence modeling and the CFX built-in laminar adiabatic Flamelet model with a chemistry based on the ANSYS C1 mechanism is used for combustion modeling. The same turbulence model is used by IVLR Uni Stuttgart in TASCOM3D but while the turbulent Prandtl and Schmidt numbers are set to $Pr_t=Sc_t=0.9$ in CFX, they are set to $Pr_t=Sc_t=0.7$ in TASCOM3D.

Regarding the normalized pressure profile shown in Fig. 3 it is notable that the CFX results have a profile which is concave with respect to the origin just as the LES results by CERFACS while the other RANS results tend to show convex curves. Furthermore, CFX shows the highest normalized pressure loss. This indicates that there is a comparatively strong heat release in the first part of the chamber which then decreases continuously. This is however not the trend shown by the experimental data. The absolute pressure profile (see Fig. 2) shows that CFX computes a pressure level which compares well with the other simulation results but which is more than 1 bar below the measured one.

In comparison with the available test data for the specific wall heat flux shown in Fig. 4, it can be seen that the CFX simulation gives one of the best estimations of the measurement data. The profile is not matched perfectly but the general level fits quite well. However, if the turbulent Prandtl and Schmidt numbers would not have been set to $Pr_t=Sc_t=0.9$ but to $Pr_t=Sc_t=0.7$ instead just as for TASCOM3D, the agreement would be worse: There would be a significant overestimation of the wall heat flux. This example shows how important it is to discuss these numbers.

The maximum heat flux value in the throat region for CFX is about 8 MW/m^2 which seems to be quite low considering that the other simulation results range between 6 MW/m^2 and 22 MW/m^2. This is an issue which should be adressed in possible future work.

The maximum temperature in the CFX result is 3366 K, i.e. about 80 K below the equilibrium value. However, as visualized in the temperature contour plot in Fig. 5, the CFX temperature is quite high compared to the other flamelet simulations and to the LFA simulation with equilibrium chemistry, although the CFX flamelet model also uses a Beta-PDF to account for turbulence chemistry interaction. This is an interesting differ-

ence which might be worth some further investigations.

The present results stem from a first attempt to simulate this test case with CFX, i.e. the invested efforts are very low, most probably much lower than for the other simulations of this comparison. At the time being it is not clear whether this approach will be pursued. Nevertheless, it has been decided to provide the results of this first attempt for comparison as good example of how a simulation result can agree well with a part of the available test data (here the wall heat flux profile) but disagree with another part and thus leave several open questions. In order to adequately assess the quality of a simulation, it is necessary to not only consider a part of the available test data but all of it. The well-known Penn-State test case [12] is a good example for a test case where several CFD results have been published by different authors without comparing the computed chamber pressure to the measured one although it was given in the test case description. As turned out at some point, it is not possible to reach the measured chamber pressure with the given boundary conditions for that test case. This shows: If the simulation results are not challenged from every possible point of view, defects (either in the simulation results or in the test data) will remain undetected.

4.4. *Japan Aerospace Exploration Agency, JAXA*

First characteristic of JAXA's simulation is using the skeletal chemical reaction set of CH_4/O_2 proposed by DLR, which includes 21 species and 97 chemical reactions. The chemical species changes, i.e., the occurrence of recombination of H_2O and CO_2, in the thermal boundary layer where the temperature decreases for the heat loss at the combustion chamber wall. The chemical reaction set needs to recreate the changes of species and reaction rate. As shown in the results of other group, the chemical equilibrium model, which is workable in H_2/O_2 combustion, is not adequate because CH_4/O_2 reaction is relatively slow. Although the wall heat flux in the nozzle is not the evaluation object, the change of chemical species in the nozzle is also very important for the prediction of the wall heat flux. If we use the flamelet model, the pressure dependent and heat loss effect should be included in the flamelet table.

Second characteristic is the three-dimensional calculation. If there is a distribution in the circumferential direction, the total heat fluxes are different between the two-dimensional axi-symmetric and three-dimensional calculation. The total heat flux affects the prediction of the combustion pressure. If we use two-dimensional axi-symmetric calculation, the combustion pressure in simulation will become lower than that in experiment. For the next step, the comparisons of the wall heat flux in the circumferential direction between the simulation results and experimental data should be performed.

The differences between the simulation results and experimental data are described as follows;

1. The combustion pressure in the simulation results is lower than that in the experimental data.

2. The pressure in the simulation results does not show a flat profile at the end of the combustion chamber.

3. The simulation results of the wall heat flux underestimate the experimental data near the faceplate.

4. The simulation results of the wall heat flux overestimate the experimental data at the end of the combustion chamber.

Item 1, 2, and 4 indicate that the flame length in the experiment was shorter than that in the simulation. Therefore, the reaction in the experiment is faster than that in the simulation. There are some solutions for the physical model to accelerate the reaction

in the simulation. To achieve both of the fast reaction and the resolution of Item 3, we will focus on the mixing between the fuel and oxidizer near the face plate. For the next step, the effects of the unsteadiness of flow field and the turbulence combustion models will be revealed for the mixing near the face plate.

4.5. *The European Centre for Research and Advanced Training in Scientific Computation, CERFACS, France*

A 3D large eddy simulation of the whole single element GCH_4/GOX combustion chamber characterized at TUM has been performed in this work, followed by a chained calculation of the chamber structure temperature distribution using the heat fluxes provided by the LES. The LES has been carried out by assigning the experimental temperature profile at the chamber walls with an isothermal boundary condition. The wall heat flux has been calculated and has been used as boundary condition for the thermal solver: the temporal evolution of temperature within the solid has been estimated.

For the LES, the computational domain has been discretized with a fully tetrahedral unstructured mesh of about 50 millions cells. Particular attention has been put on the flame zone refinement, especially in the post-tip zone, which has been discretized with 20 cells. Regarding boundary conditions, it must be pointed out that the walls have not been resolved and chamber walls have been modeled with isothermal wall laws, using an improved formulation that couples the velocity and temperature profiles to take into account the interaction between the strong temperature and density gradients in the boundary layer [13]. The LES has been performed by means of the AVBP solver [8, 14], using the TTGC numerical scheme [16], Smagorinsky model [17] for the subgrid stress tensor, fixed values for turbulent Prandtl and Schmidt numbers and a fully resolved turbulence/combustion interaction. The semi-analytical scheme of Lu [18] has been used to describe CH_4/O_2 combustion, together with a ten steps chemical sub-cycling.

The thermal simulation has been performed using the AVTP solver. The solid domain has been discretized with a fully tetrahedral mesh of 33 millions cells and initialized at ambient temperature. The whole three seconds of the experiment have been simulated.

In such configuration the physical mechanisms which are present just downstream of the post-tip have been found to strongly govern the flow and flame structure in the close injector region, and a process of analysis and improvement of the mesh resolution was necessary to ensure a correct solution. The actual mesh (which will be called fine mesh) has been compared with a coarser one (which will be called coarse mesh), where the post-tip has been discretized with 10 cells. With the fine mesh there is the presence of a recirculation zone in the post-tip area, which pushes the reactant jets closer forcing them to mix. This backflow zone is filled with hot gases and has a direct influence on the flame stabilisation mechanism: the recirculation zone confines the flame on the oxygen side and dilutes the CH_4 flux with burned gases, limiting the heat release which reaches its maximum later downstream, when its position aligns with the stochiometric mixture fraction isosurface. On the other hand, with the coarse mesh, the poor resolution causes the recirculation zone in the post-tip area to almost disappear: the reactants quickly diffuse after the post-tip, aligning with the stoichiometric mixture fraction isosurface and creating favorable conditions for combustion, leading to a maximum of heat release. The flame is less strained and the hot products are free to expand radially, generating a thick flame which pushes the CH_4 jets towards the wall and leaves the flow free to generate large recirculation zones between the two jets.

The comparison with experimental data shows a linked effect of underestimation of chamber pressure and overestimation of wall heat fluxes, as shown in Fig. 2 and 4. Re-

garding the pressure evolution one can however notice from Fig. 3 how the global trend is well captured, denoting: a peak in the immediate vicinity of the faceplate (end of the corners recirculation zone and impact of the flow to the wall), a gradual decay in the flame zone due to flow acceleration, a plateau (low pressure gradient) in the zone close to the end of the chamber (end of the combustion process, which indicates a correct prediction of the flame length).

Regarding the wall heat flux one can see two different but linked effects: first an overshoot in heat flux is present, denoting temperatures in the fluid higher than the expected ones close to the walls, due probably to a lack of resolution of the flow and flame shape downstream of the refined zone. Second, in the zone near to the end of the chamber, a smaller but still important overestimation of the heat flux is visible, suggesting that even in zones with no strong flame/wall interaction the heat fluxes are overestimated. This is probably caused by the lack of resolution of the chamber walls boundary layer, that are treated with wall laws using values for y^+ around 600. This effect can in turn be in part the cause of the overestimation of the fluxes in the central part of the chamber, where really high differences in temperature appear in a not sufficiently refined zone. Ongoing study and further work are and will be focused mainly on the influence of the mesh on the flame structure and of the wall resolution on heat losses, to understand the reasons of the wall heat flux overestimation. In particular wall laws will be tested with different values of y^+ and different element types, such as prisms, which allow for the resolution for this highly non isotropic zone.

4.6. *Technische Universität München, Institute of Thermodynamics (TD)*

The work conducted at the Institute of Thermodynamics during the summer program is focused on methods of low computational effort. The background of this approach is the cost effective computation of mean flow fields suitable for thermoacoustic stability analysis. Thus capturing governing flow features is more relevant than resolving the flow in high detail. This work is just an initial, preliminary approach, to this type of setup and the results presented within the scope of this report are to be considered as intermediate output of ongoing work. A more detailed discussion is given in [19].

In a first step, stationary RANS computations using the k-ω-SST model are conducted. Combustion is modeled via a steady diffusion flamelet approach to avoid costly kinetic computations. In addition the geometry is approximated by a two-dimensional axis symmetric configuration. Injector, chamber and throat radii are chosen to preserve the respective crossectional area. More information on the setup can be found in Tab. 1.

For comparison to experimental data, wall heat fluxes and pressure profiles are given in Fig. 4 and 2 respectively. It can be stated that while the qualitative tendencies of the experimental data are roughly met, pressure as well as wall heat flux are underestimated. Especially the combination of the last two points is of importance. While an increasing wall heat flux tends to decrease the chamber pressure, just the opposite is true for the heat release. Thus the underprediction of wall heat flux appearing together with underpredicted chamber pressure marks a significant lack of heat release.

The qualitative evolution of pressure is shown in Fig. 3 via its normalized value. While the relative global pressure drop across the chamber is met, the shape of the profile is more complex in the experiment. Especially the flattening of the profile at the last two measurement positions, indicating completed combustion, is not captured by the simulation. Besides, the numerical determined maximum value of the normalized pressure lies below the experimental one.

The temperature distribution shown in Fig. 5 indicates that the flame persists down-
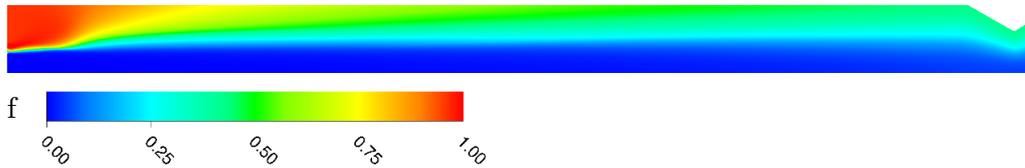
FIGURE 6. Mixture fraction.

stream until the chamber exit. This is supported by the structure of the mixture fraction, which is shown in Fig. 6. There a strong stratification at the chamber exit exists, suggesting poor mixing as main reason for the uncompleted combustion and underpredicted heat release.

Compared with the results of other groups, the computed wall heat flux is lower. However, the deviation from the experimental data lies within the range of the other simulations. In contrast, the offset in pressure level stands out. While the difference in the relative pressure distribution remains comparable low (cf. Fig. 3), the computed absolute values differ by about 1.5 bar (cf. Fig. 2). From the different setups (cf. Tab. 1) no obvious reason appears for this deviation. While the exact setup is not met by any other group, the Airbus DS CFX-Approach is quite similar. It seems unlikely that in a flamelet approach the reaction mechanism accounts for that significant differences in the results.

Altogether the intermediate results indicate a significant underprediction of mixing inside the chamber. Thus in further work the accuracy of this aspect has to be increased. The focus will be placed on the corresponding turbulence closure. This may include the adaption of RANS turbulence parameters, the turbulence model or even the advance to a higher degree of resolved scales, e.g. via Detached Eddy Simulations (DES).

4.7. *Universität Stuttgart, Institute of Combustion Technology for Aerospace Engineering (IVLR)*

The presented results are performed using the inhouse code TASCOM3D for a steady three-dimensional simulation of a quarter of the chamber. In contrast to most other presented simulations the injector is fully resolved using low-Reynolds turbulence models which results in the finest post tip resolution of all simulations. The grid consists of 835,000 cell volumes and is block-structured. The grid resolution in the axial direction is rather coarse while the radial number of cells, compared to the other structured grids in this report, is quite high, see table 1. TASCOM3D utilizes high order spatial discretization up to fifth order using MLP^{ld}. Furthermore, laminar finite-rate chemistry with a kinetic mechanism consisting of 21 species and 97 reactions is used. The turbulent Prandtl and Schmidt numbers are each set to 0.7. This is the lowest value of all the presented RANS simulations.

The predicted normalized wall pressure profile, depicted in Fig. 3, is well within the other simulations' results. The overall relative pressure drop is underpredicted and the zero gradient between the last two measurement points is not reproduced. The pressure is underpredicted by about 1 bar which is due to a bad combustion efficiency, as is shown in the individual report.

The wall heat fluxes are overestimated by the simulation, which is the case for all simulations, see Fig. 4. The qualitative agreement with the measured values has some shortcomings as well. The simulated heat flux rises later than the measured one and the flattening of the profile is not reproduced properly by the simulation. This can be best explained by shortcomings concerning in the prediction of the recirculation zone

and the flame position. Besides these shortcomings, it is still unclear how to compare the one-dimensional heat flux measurements with the two-dimensional results from the simulation. In the presented case, the values at the center line were chosen (maximal values) since this is also the measurement location. It was observed, that there is a significant variation of the wall heat flux in the circumferential direction.

As mentioned above, the presented simulation was performed using 0.7 for the turbulent Prandtl and Schmidt numbers. It was shown in the individual report that these numbers have a strong impact on the quantitative values of both pressure and wall heat flux. This remains an open issue and should be addressed further.

Future work for the combustion chamber will include unsteady simulations on two- and three-dimensional grids. From unsteady simulations, better predictions of the mixing processes and thus combustion is expected. Furthermore, a smaller dependency on the turbulent Prandtl and Schmidt numbers is anticipated for those simulations.

4.8. *Universität der Bundeswehr München, Thermodynamics Institute*

The contribution of the UniBW is a 2-dimensional unsteady RANS simulation that is performed using the open-source CFD platform OpenFOAM. We use the grid that has been defined during the summer program to allow for a better comparison of the different approaches. It is axisymmetric and comprises $45 \cdot 10^3$ cells, which is too coarse to guarantee grid-independent results.

The focus of this work lies on the validation of a tabulated chemistry approach to predict heat losses in rocket combustion chambers at elevated pressures. This has the advantage that the huge computational cost of solving the chemistry kinetics during run-time can be avoided and complex mechanisms can be used at a reasonable effort. Hence, we employ a non-adiabatic flamelet/progress variable method to model turbulent combustion with wall heat loss. In the flamelet concept, the turbulent flame is assumed to consist of small laminar diffusion flames [20]. This assumption is justified for sufficiently high Damköhler numbers, meaning that chemical time scales are small compared to convective time scales. Moreover, chemical reactions are assumed to occur in thin reaction layers that are small compared to the turbulent length scales. The local flame structure can then be calculated in a pre-processing step using finite-rate chemistry, stored in a flamelet library and coupled to the turbulent flow using few parameters. During run-time, equations are solved for those controlling parameters and the corresponding thermodynamic quantities and species mass fractions are retrieved from the library. In the present work, we use the mixture fraction together with a flame progress variable and the absolute enthalpy.

The influence of turbulence on the chemical reactions is modelled with a presumed β-shape probability density function. Turbulence is described with the Launder-Sharma k-ε model [8] and the turbulent Schmidt- and Prandtl number is set to $Pr_t = Sc_t = 0.85$. The walls are resolved and no additional wall modelling is applied.

The profile of normalized pressure in Fig. 3 compares well to the results of the other codes, but neither the steep pressure increase at the beginning of the chamber, nor the plateau region at the end of the chamber is satisfactorily reproduced. The pressure plateau at the chamber end indicates completed combustion. However, in our numerical simulation, the flame is very long, as can be seen in Fig. 5 and the maximum temperature is reached just shortly before the nozzle. We observe unburned oxygen at the nozzle exit, meaning that the reaction is not completed.

The absolute pressure (Fig. 2) is underpredicted, while the wall heat flux depicted in Fig. 4 is overestimated compared to the experimental data. The numerical wall heat flux

features a peak at the end of the recirculation zone, as can be seen in the experimental data as well. Further downstream the wall heat flux increases to 4.5 MW/m^2 where it exhibits a short plateau region and further increases thereafter. At the end of the chamber a second plateau of approximately 10.5 MW/m^2 is reached.

5. Conclusions

CFD simulations of the flow and combustion in a single-element GOX/CH$_4$ rocket combustor were performed. The results achieved by seven research groups employing different models implemented in different tools were compared against each other and against experimental data. The experimental results were not distributed to the groups a priori as to facilitate a 'blind test'. The results show considerable differences with regard to the prediction of the flow field and the validation parameter.

Almost all simulations underpredict the measured combustion pressure and combustion efficiency while they overestimate the wall heat flux. The only exception is the simulation by TUM-TD, which underpredicts the heat flux and the combustion pressure. It can be concluded that for the accurate prediction of the wanted validation and design parameter the heat transfer to the wall, the combustion process and the mixing process must be predicted with a certain accuracy.

The results achieved stem from simulations with greatly varying degree of computational effort. However, none of the simulations predict the validation parameter sufficiently. A clear trend of improved results for the validation parameter with higher degrees of fidelity in the computational simulations could not be observed. Additional effort has to be undertaken to improve the solutions of the individual groups.

To understand better the influence of 3D effects from the rectangular cross section of the combustion chamber, further investigations without the assumption of an axissymmetric geometry are going to be performed. Then a conclusion can be drawn whether the considerably less computationally expensive 2D simulation can predict the validation and design parameters within an acceptable range of accuracy.

It is still an open question whether a steady state simulation can be used to accurately simulate a test case that is based on an experiment which is inherently transient. A test case that runs under steady state conditions from an experimental point of view should help answer this question.

Acknowledgments

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