Numerical Investigation of Flow and Combustion in a Single-Element GCH_4/GOX Rocket Combustor

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The flow and combustion in a GCH_4/GOX single-element rocket combustor is analysed by several groups using different numerical models and tools. The tools and simulation setups vary with respect to modeling fidelity and computational expense. A short overview of the tools and the individual simulation setups is given. The focus of the paper is the comparison of the results obtained by the different groups as well as with experimental data. This encompasses the study of specific features of the combustor flow among the different simulations, as well as the validation with typical rocket engine design and performance parameters, such as wall heat flux and combsution pressure, gained from hot firing tests.

Nomenclature

k	turbulent kinetic energy
q	square root of turbulent kinetic energy
T	temperature
$y+$	dimensionless wall distance
ε	turbulent dissipation
ω	specific turbulent dissipation

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Acronyms

ADS	Airbus DS GmbH
CAD	Computer Aided Design
CEA	Chemical Equilibrium Composition and Applications
CERFACS	Centre Europeen de Recherche et de Formation Avancee en Calcul Scientifique
CFD	Computational Fluid Dynamics
GCH_4	Gaseous Methane
GOX	Gaseous Oxygen
IMFT	Institut de Mecanique des Fluides de Toulouse
IVLR	Institut für Verbrennungstechnik der Luft- und Raumfahrt, Universität Stuttgart
JAXA	Japan Aerospace Exploration Agency
LES	Large Eddy Simulation
LFA	Institute for Flight Propulsion, Technische Universität München
RANS	Reynolds Averaged Navier Stokes
SFB/TRR 40	Sonderforschungsbereich Transregio 40
TCI	Turbulence Chemistry Interaction
TD	Institute for Thermodynamics, Technische Universität München
UniBw	Institute for Thermodynamics, Universität der Bundeswehr München

I. Introduction

In the design and optimisation of liquid rocket engines, computational fluid dynamics (CFD) can be used to support and substitute costly experimental test runs. One area where CFD tools are typically employed is the layout of the heat management system and the performance analysis of a rocket combustor. In order to be able to support the development process and make more educated design choices the used tools must be able to describe the different physical processes encountered in rocket thrust chambers, like fluid flow, combustion, and heat transfer. Simulations must be able to predict design parameters within a certain accuracy without being prohibitive to perform due to computational cost. In addition, to increase the level of confidence in the numerical predictions, tools and models need to be validated with experimental data over the wide range of operating conditions that occur in rocket combustors.

In the framework of the research program SFB/TRR 40 *Fundamental Technologies for the Development of Future Space-Transport-System Components under High Thermal and Mechanical Loads*, the Institute for Flight Propulsion at the Technische Universität München conducted several hot firing tests of a lab-scale single-element rocket combustor using GCH_4/GOX as propellant combination. The test data has been made available for validating numerical tools and models in a dedicated test case.[1]

A first effort to simulate this test case has been made during the 2015 SFB/TRR 40 Summer Program. Different research groups simulated the test case in a 'blind test', i.e. without knowledge of the validation data, using their individual tools. The results showed significant deviations amongst the simulations by the different participating groups and in comparison to the test data.[2] The present paper presents updated results of the common effort to improve the numerical predictions of combustion and heat transfer processes in rocket engines. Specific features of the flow fields and the combustion process predicted by the different tools are presented and compared. The focus is on the prediction of design and performance parameters relevant in rocket engine design, i.e. combustion pressure, wall heat flux and combustion efficiency.

As part of the effort, studies of more specific aspects of the modeling approaches have been conducted in separate publications. The aspect of turbulence modeling is discussed in the publication by Chemnitz et al.[3] The modeling of chemistry and turbulence chemistry interaction is presented by Maestro et al.[4] The efforts to simulate the test case using Large Eddy Simulation (LES) are presented by Müller et al.[5]

II. Test Case Description

The test case used for the validation efforts is described in Ref. 1. 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. After the combustor the hot gas is expanded to ambient pressure in a

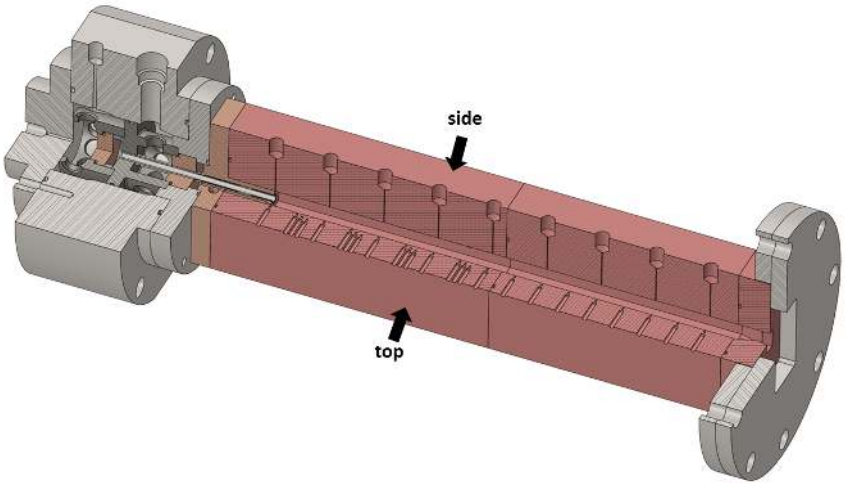

Figure 1: CAD model of the combustion chamber.

convergent-divergent nozzle. A CAD model of the combustion chamber is shown in figure 1.

The combustor is lab-scale with a total length of 310 mm and a square cross section of 12x12 mm. The contraction ratio is 2.5, which is close to actual flight hardware (Vulcain: 2.5, Aestus: 2.38). The operating point presented has a nominal oxidiser to fuel ratio of 2.6 and a chamber pressure of 20 bar. As propellants gaseous methane and gaseous oxygen are used.

The combustion chamber and the nozzle are made of oxygen-free copper and the assembly is capacitively cooled. Due to the type of cooling, the chamber can only be operated for a limited time period per hot firing test. In a typical test run the combustor is therefore only operated for three seconds. The nature of the test case therefore is transient. For comparison between test data and computational predictions, the wall heat flux and the combustion pressure from the experiment are available. The experimental wall heat flux is reconstructed from the readings of thermocouple clusters, which are distributed in axial direction along the top wall, according to the method described in Ref. 6. Combustion pressure is measured with pressure transducers that are lined up in axial direction along the combustor's side wall.

III. Tools and setup description

In this section a brief description of the different numerical tools used by the individual groups is given and the different setups in terms of mesh and employed models are described. There were seven groups contributing their results. An overview of some key models and parameters used in the simulation setups is given in table 1.

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

The Institute for Flight Propulsion performed a RANS simulation of the test case using the commercial CFD code ANSYS Fluent. A quarter of the combustion chamber was simulated with a mesh consisting of 2.5 million computational cells. Symmetry was assumed along two perpendicular planes through the combustor. As turbulence model a two-equation k-ε model[7] was used with a two-layer approach in the wall near region, allowing a resolution of the wall with a $y+$ smaller than one. As combustion model a frozen flamelet was used with an assumed shape beta-pdf approach to model turbulence chemistry interaction. Frozen flamelet here refers to a flamelet modelling approach, where flamelets are calculated under adiabatic conditions and enthalpy loss/gain is modeled in a second step by extracting or adding heat while keeping the calculated gas composition fixed. This means the heat extracted through the combustor wall does not impact the composition of the hot gas, only the temperature. The impact of this assumption will be investigated further in the future. As chemical kinetic mechanism the scheme presented by Slavinskaya et al.[8] was used. Turbulent Prandtl and Schmidt numbers were set to a constant value of 0.9 and 0.6 respectively.

B. Airbus DS GmbH (ADS)

The Airbus DS GmbH contributed a simulation of the test case performed with their in-house tool Rocflam3. Rocflam3 is a RANS CFD tool for structured multiblock grids that has been specifically developed for the simulation of flow and combustion in rocket engines and has already been applied in the simulation of methane rocket combustors.[9] The simulation presented here was performed on the same mesh as the simulation by the LFA. A low reynolds version of a k-ε model devloped by Launder and Sharma[10] was used for modeling turbulence. Chemistry was modeled using an equilibrium chemistry approach with nine species and an assumed pdf in beta shape to simulate TCI. This is the only approach used in this comparison, that does not explicitly require a kinetic chemistry model. Turbulent Prandtl and Schmidt numbers were set to 1.2 and 0.9 all throughout the domain. Where the value of 1.2 for the turbulent Prandtl number is the highest one among all different setups.

C. Institut für Verbrennungstechnik der Luft- und Raumfahrt (IVLR), Universität Stuttgart

The Institut für Verbrennungstechnik der Luft- und Raumfahrt performed a simulation using their in-house CFD code TASCOM3D. The tool has also previously been used in the simulation of heat transfer processes of gas/gas injector rocket engines.[11] The mesh used in this simulation consists of 0.8 million cells and is therefore smallest of all grids used. It is about three times smaller than the second smallest used by the LFA and ADS. Turbulence is modeled using a q-ω model, which allows the resolution of the wall up to $y+$ values below one. The combustion process is modeled using a laminar finite rate chemistry approach with the chemical kinetic scheme by Slavinskaya et al.[8] Turbulent Prandtl and Schmidt numbers were set to 0.9 and 0.7 all throughout the domain. A study of the impact of these two parameters for TASCOM3D was presented in Keller.[12]

D. Institute for Thermodynamics (UniBw), Universität der Bundeswehr München

The Institute for Thermodynamics at the Universität der Bundeswehr München used an adapted version of the CFD package OpenFOAM[a] to simulate the test case. OpenFOAM is a fully parallelized open-source CFD software that has been extended by the Universität der Bundeswehr München (UniBW) to allow for simulations of real gas flows and reacting flows using various combustion models. OpenFOAM is a widely used platform and has been applied to simulate a multitude of physical processes. The code uses a pressure-based solution approach for transonic flows based on the compressible version of the PISO method and employs second order linear differences for spatial discretization. Recently, the framework has been used to study both non-reacting[13,14] and reacting[15] flows at rocket-like conditions. In the present contribution, the combustor was simulated with large eddy simulation resolving the larger turbulent scales, while closing the subgrid-scale turbulence using the Vreman model.[16] The frozen flamelet model with the presumed PDF approach as described above is employed as combustion model. The local flame structure is represented by a flamelet library that has been generated using the reduced methane mechanism of Slavinskaya containing 21 species and 97 reactions.[8] A power law is used for the molecular viscosity and the thermal conductivity is computed using the viscosity, specific heat capacity at constant pressure and a constant molecular Prandtl number. The coefficients have been fitted to the Chapman-Enskog theory. On the subgrid level, turbulent Prandtl and Schmidt numbers are set to 0.7 and 0.7 all throughout the domain. The computational domain encloses the full chamber, therefore no symmetry is assumed. The mesh consists of 90 million cells with high grid density close to the wall and is by far the largest grid used in this comparison.

E. Japan Aerospace Exploration Agency (JAXA)

The Japan Aerospace Exploration Agency performed a RANS simulation of a quarter of the investigated combustor using the commercial CFD software CRUNCH-CFD. The simulation was performed on a mesh consisting of 4 million computational cells. As turbulence model a two-layer k-ε model was used resolving the wall to $y+$ values smaller than one. As combustion model a laminar finite rate chemistry employing the kinetic chemistry scheme described in Slavinskaya et al.[8] was used. The turbulent Prandtl and Schmidt numbers were set to a constant values of 0.9 and 0.9.

[a] www.openfoam.com

F. Institute for Thermodynamics (TD), Technische Universität München

The Institute for Thermodynamics performed a RANS simulation of the test case using the commercial CFD code ANSYS Fluent. The setup is very similar to the setup used by the LFA. The main differences are the grid and the modeling of the transport properties as well as the inflow boundary conditions. The mesh used by the TD group has 4.5 million cells compared to the one used by the LFA with 2.5 millions cells. The calculation of the transport properties by the Institute for Thermodynamics is based on the model described in Ref. 17. The LFA in contrast uses a transport model based on Ref. 18. TD uses an inflow profile for velocity and turbulence based on a simulation by JAXA, while LFA simply uses block profiles.

G. Centre Européen de Recherche et de Formation Avancée en Calcul Scientifique (CERFACS)

The CERFACS research group contributed a LES simulation of a quarter of the combustion chamber using their in-house code AVBP. The domain was resolved with 60 million cells, which makes this the most highly resolved simulation, especially in the injector near region. The turbulence on the subgrid level is modeled using the Smagorinsky model.[19] A finite rate chemistry model is used for simulating the combustion process. A reduced chemical scheme by Lu[20] is used to capture combustion kinetics. CERFACS is the only group using a kinetic scheme other than the scheme by Slavinskaya et al.[8] Rather than modeling turbulence chemistry interaction it is fully resolved on the mesh. Turbulent Prandtl and Schmidt numbers were set to 0.7 and 0.7 all throughout the domain on a subgrid level. As only group CERFACS modeled the nozzle, where no experimental heat flux data was available, as adiabatic. CERFACS is also the only group not resolving the wall near region with computational cells, but rather using a wall law for the calculations. The $y+$ value of the cells next to the wall is around 40.

IV. Results

In the following the results of the simulations conducted by the different participating groups are discussed. These are the up to date results obtained by the individual groups without any restrictions on modeling or computational expense. First, the prediction of the flame structure and the combustion process are discussed and compared amongst the groups. Then the computed wall heat fluxes are considered, regarding the three dimensional structure as well as the agreement with experimental data. At last, the predicted pressure distribution along the axial direction of the chamber is presented. The results are compared with each other as well as with experimental data for validation.

A. Combustion process and flame structure

In the test case configuration, as in typical rocket engines, the propellants enter the combustion chamber non-premixed. The injector elements are responsible for mixing the fuel and the oxidiser sufficiently fast. In this case a single coaxial-type injector is used.

As presented in section III the different tools employ different strategies for modelling chemistry and turbulence chemistry interaction. The resulting temperature fields are shown in figure 2. In general it can be seen that a hot zone is created in the recirculation zone of the post tip. From there the reacting zone is expanded and the flame broadens towards the downstream end of the combustor. Comparing the individual fields, one can see some distinct characteristics of the different flames.

The two simulations using a laminar finite rate chemistry model (IVLR and JAXA) feature a relatively thin very hot zone which starts at the injector tip and then widens progressively through the chamber. As the hot zone gets closer to the wall, a visible temperature layer is build up due to the heat flux through the chamber wall. The simulations by LFA, ADS, and TD do not feature such a distinct hot zone but have a more broad temperature distribution, which is probably related to the use of the beta-pdf model for TCI, which tends to 'smoothen' the temperature field. In these simulations the hot zone reaches the wall earlier in the chamber and the distinct temperature layer starts closer to the faceplate. The simulation performed by CERFACS shows a quickly opening flame that touches the wall in the first third of the chamber. Only a very small temperature layer is formed. In contrast, in the simulation by the UniBw the hot zone never gets close to the wall.

Furthermore, in figure 2 the maximum temperatures occurring in the individual simulations are given.

Group	LFA	ADS	IVLR	UniBw	JAXA	TD	CERFACS
Tool	Fluent	Rocflam3	TASCOM3D	OpenFoam	CRUNCH-CFD	Fluent	AVBP
Equations	RANS	RANS	RANS	LES	RANS	RANS	LES
Geometry	3D/Quarter	3D/Quarter	3D/Quarter	3D/Full	3D/Quarter	3D/Quarter	3D/Quarter
Mesh Cells	$2.5 \cdot 10^6$	$2.5 \cdot 10^6$	$0.8 \cdot 10^6$	$90.0 \cdot 10^6$	$4.0 \cdot 10^6$	$4.5 \cdot 10^6$	$60.0 \cdot 10^6$
Turbulence Model	k-ε Two-Layer	k-ε Low-Re	q-ω	Vreman Subgrid	k-ε Two-Layer	k-ε Two-Layer	Smagorinsky Subgrid
Combustion Model	Frozen Flamelet	Equilibrium Chemistry	Finite Rate Chemistry	Frozen Flamelet	Finite Rate Chemistry	Frozen Flamelet	Finite Rate Chemistry
TCI Model	β-PDF	β-PDF	Laminar	β-PDF	Laminar	β-PDF	Resolved
Chemistry	21 Species 97 Reactions	9 Species	21 Species 97 Reactions	21 Species 97 Reactions	21 Species 97 Reactions	21 Species 97 Reactions	13 Species 73 Reactions
$\mathrm{Pr_t}/\mathrm{Sc_t}$	0.9/0.6	1.2/0.9	0.9/0.7	0.7/0.7 Subgrid	0.9/0.9	0.9/0.6	0.7/0.7 Subgrid

Table 1: Model and setup overview.

The adiabatic flame temperature at equilibrium as calculated with CEA is 3444 K. This value can vary slightly depending on the thermodynamic data used and the product species included. It is a good indicator of the maximum temperature that can occur in a combustion process. Most simulations show temperatures close to that value. Exceptions are the IVLR simulation, which is about 100 K above the equilibrium temperature, and the UniBw simulation, which is about 300 K below. In the UniBw simulation this is only true for the averaged maximum temperature due to strong fluctuations in the combustor flow. The instantaneous maximum temperature actually does get close to the adiabatic Value with 3365 K.

Figure 3 shows the radial position of the stoichiometric mixture fraction. Three different types of contours can be observed. The stoichiometric contours predicted by the LFA and TD simulations, with a very similar setup, close inside the combustor, i.e. they cross the chamber axis. Most other simulations (ADS, JAXA, IVLR, UniBw) predict a stoichiometric contour that is not closed in the combustor, but leaves the domain through the nozzle exit. This is probably related to the fact that LFA and TD use the lowest value for the turbulent Schmidt number as well as a k-ε turbulence model, which has shown to predict a stronger mixing compared to the ω-based models.[3] In contrast the stoichiometric contour predicted by CERFACS opens quickly and touches the wall at about half of the chamber length.

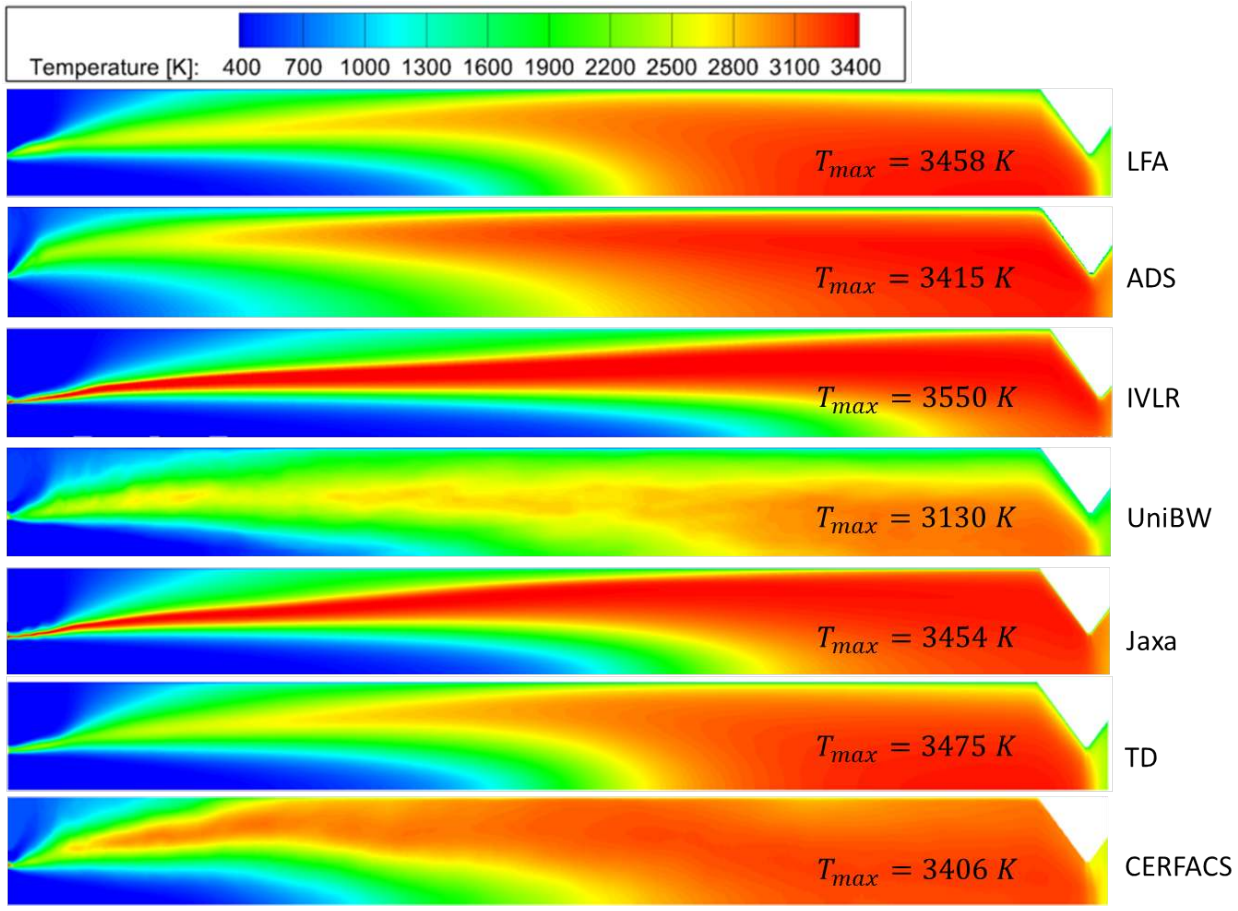

Figure 2: Predicted temperature fields in the combustor.

B. Prediction of wall heat flux

Predicting the heat conducted through the combustor wall is essential for the design of a rocket's thermal management system. In the case of the presented combustor the hardware features a square cross section. The assumption of axial symmetry that can often be made in rocket engines is not valid and the wall heat flux shows a strong variation along the circumference. The wall heat flux is evaluated at three distinct locations, the top, the side, and the corner, where the corner is defined as a location 1 mm from the side

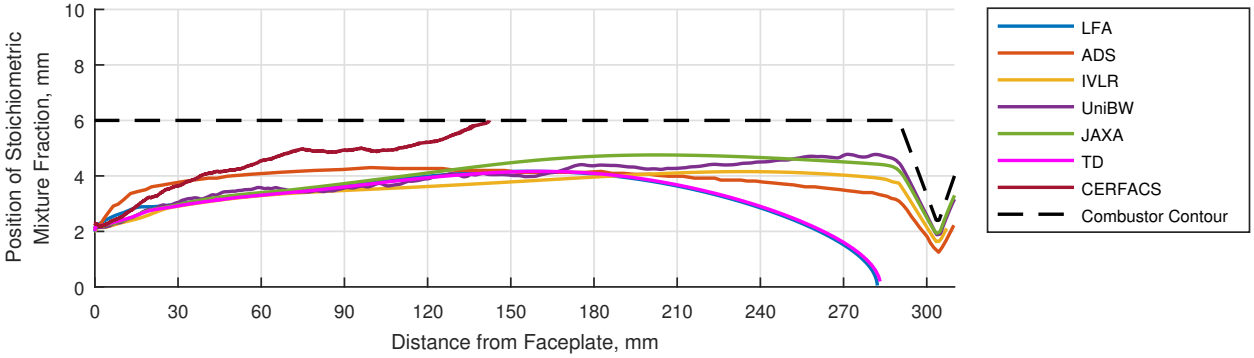

Figure 3: Contour of stoichiometric mixture fraction.

wall. The circumferential average is compared to the reconstructed experimental heat flux.

The experimental heat flux values have been determined from thermocouple readings using an inverse heat conduction problem. The determination procedure is described in Ref. 6. No circumferential heat flux distribution is given in the experimental data. Instead an averaged heat flux was used in the reconstruction process. Therefore the experimental values are compared to the circumferential average of the simulations. Figure 4 shows the predictions of the average heat flux by the different participating groups in comparison with the data determined from the hot firing test.

The experimental data shows a steep rise in the injector near region. After a short drop, that is likely related to a recirculation zone near the faceplate, the heat flux rises continuously until it reaches a plateau near the end of the combustion chamber.

The two laminar finite rate chemistry simulations (IVLR and JAXA) again show a similar trend. Both do not predict the heat flux plateau at the end of the combustor, in contrast to the other simulations. This is consistent with the presented temperature fields, which show a continuously developing temperature layer in the near wall region. The JAXA simulation predicts a steeper heat flux rise in the beginning, but at about half way through the combustor the heat flux predicted by the IVLR becomes higher. This is against expectations due to the fact that the turbulent Schmidt number in the IVLR simulation is lower (0.7 compared to 0.9), which usually promotes a stronger mixing and thus an earlier heat flux rise. A possible reason for this effect is the use of the different turbulence models. While IVLR uses a ω-based model, JAXA uses an ε-based one which has been shown to predict a stronger mixing.[3] The ADS simulation overestimates the heat flux in the first part of the chamber substantially, but comes closer to the experimental data towards the combustor end. ADS uses a combustion model that assumes local chemical equilibrium in every computational cell explaining the comparatively high values for the heat output. The same tendency is seen in the CERFACS simulation to a lesser extent. The flame predicted by CERFACS opens fairly early in the chamber and gets very close to the wall forcing a high heat flux through the combustor wall. The predicted heat flux values of JAXA and TD show good agreement with the experimental data except for the prediction of the steep heat flux rise in the beginning, which is only captured by the CERFACS and ADS simulation. The LFA simulation also does not capture the steep heat flux rise in the beginning. It does however start to overestimate the heat flux fairly early in the chamber, at about a fifth of the chamber. The predicted plateau value is above the experimental one. The overestimation of the heat flux in comparison to the TD simulation is most likely caused by the used models for the calculation of the transport properties.

Figure 5 and figure 6 show the heat flux along the top and side wall of the combustion chamber. For most simulations the values of top and side are similar in the chamber but differ in the nozzle due to the converging top wall. The ADS simulation is the only simulation that shows notable differences in the two fluxes. Figure 7 shows the heat flux in the corner of the simulation. Comparing the heat flux in the corner to the top heat flux it can be seen that in general the corner heat flux is predicted to be lower. For most simulation it is lower between two to six times.

It can be seen from figure 4 that the heat flux calculated in the UniBW simulation is very low. The reason for that is currently under investigation. One point is that the resolution of the boundary layer imposes stringent requirements, which are not completely fulfilled by the present simulation, since the employed heat flux evaluation method assumes a fully resolved boundary layer. Moreover, the asymptotical behaviour of the

Vreman SGS model towards the wall, which is first order accurate instead of third order, might additionally influence the heat flux calculation. Further investigations into the issue are ongoing.

C. Prediction of axial pressure distribution

The predicted axial pressure distributions are shown in figure 8. All simulations underpredict the experimental values. In general, the too low pressure can be due to two reasons, the overprediction of the integrated heat leaving the combustor through the wall or the underprediction of the heat released by the combustion, which can be due to a too low mixing of the propellants or to a modelling assumption made. To give an idea of the combustion progress, the mass flow averaged mass fractions of oxygen in the simulations are plotted in figure 9 and the residual values of oxygen in the throat are given in table 2.

LFA	ADS	IVLR	UniBw	JAXA	TD	CERFACS	CEA
3.9 %	5.3 %	6.3 %	10.2 %	6.2 %	4.4 %	4.6 %	0.4 %

Table 2: Mass fraction of residual oxygen in throat.

In addition to the CFD simulations, a calculation of the test case using the Chemical Equilibrium Composition and Applications[17] (CEA) code was performed. The value of the residual oxygen in the throat calculated by CEA under the assumptions of a one-dimensional flow, adiabatic walls and homogenous mixing is plotted in figure 9 and given in table 2. The two simulations using a laminar finite rate chemistry (JAXA and IVLR) again show a similar trend, having a little more residual oxygen compared to the other simulations at around six percent while the other simulations are in the four to five percent range. Compared to the residual value predicted by CEA, which is at 0.4 %, these values are still high.

For the simulations by CERFACS, ADS and LFA, which all overestimate the average heat flux, an improved prediction of the heat flux could mitigate the underprediction of the wall pressure. In contrast the simulations by JAXA and TD underestimate the integrated heat flux but still do not reach the experimental pressure level, which means that there is not enough heat released. Heat release could be increased by an improved mixing, which would lower the residual oxygen. This would be consistent with the simulation done by CEA which shows a significantly lower oxygen level in the throat. In addition it will be investigated if the modeling assumption for the chemistry and TCI are the reason for the underprediction of the heat release.

V. Conclusion

CFD simulations of the flow and combustion in a GCH_4/GOX lab-scale rocket combustor were performed by different research groups. The results of these simulations are presented and compared among each other. The focus is the comparison of typical rocket design parameter, i.e. heat flux and combustion pressure, which are also available from the experiment.

All simulations are done on three-dimensional meshes, dropping previously made assumptions of axis-symmetry. The simulations vary strongly in fidelity, degree of modeling and computational expense, with the largest grid having about 90 million computational cells, while the smallest one only has about 0.8 million cells. In total seven simulations are presented, five of which are RANS simulations and two are LES.

In general, the predictions of the axial heat flux distributions vary notably among the simulations. ADS and CERFACS capture the steep heat flux rise in the injector near region but then overestimate the experimental heat flux in the rear part of the combustor. LFA and IVLR underestimate the heat flux in the beginning and then overestimate the plateau value at the combustor end. TD and JAXA underestimate the heat flux in the beginning as well, but show good agreement with the experimental value regarding the pressure plateau.

All simulations underestimate the combustion pressure. In general this can be related to an overestimation of the accumulated heat flux or an underprediction of the combustion efficiency. Some of the groups could mitigate the pressure loss by an improved prediction of the overestimated heat flux. But even the groups who capture the heat loss comparatively well still underestimate pressure. This indicates that the heat release is still not predicted sufficiently well, which may be due to a too weak prediction of the mixing or may be related to modeling assumptions made.

Compared to the 2015 SFB/TRR 40 Summer Program, where a first joint effort to simulate this test case was made,[2] the results in terms of the prediction of pressure and wall heat flux have improved. In

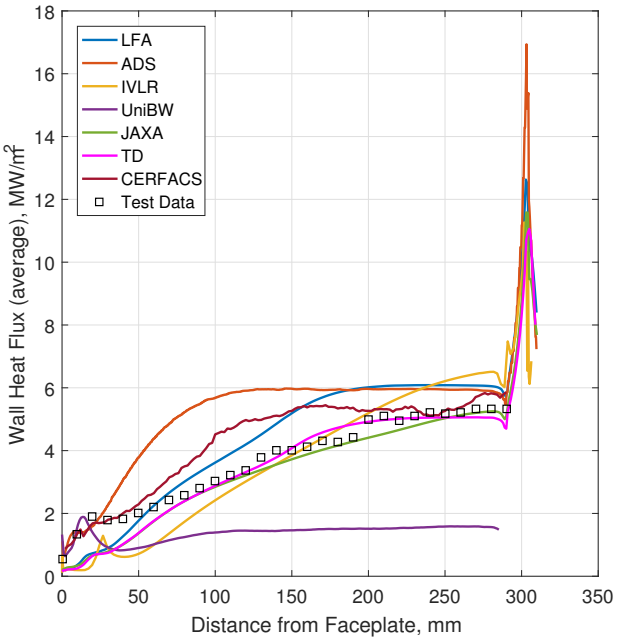

Figure 4: Heat flux averaged along circumference.

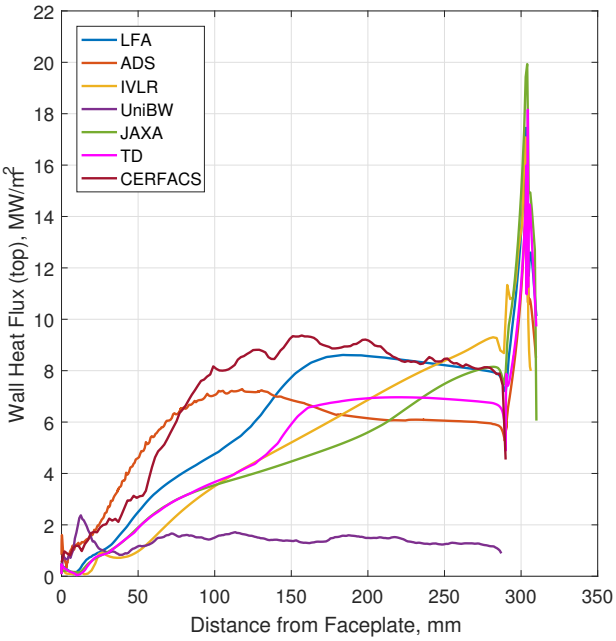

Figure 5: Heat flux along the top wall.

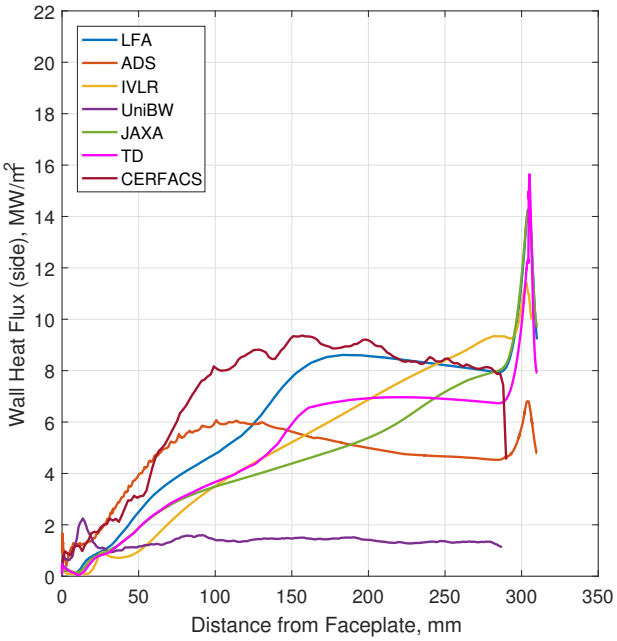

Figure 6: Heat flux along the side wall.

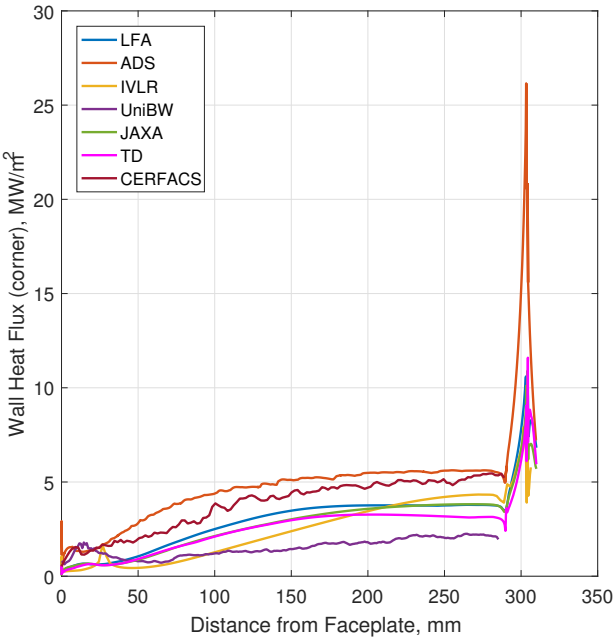

Figure 7: Heat flux along the corner.

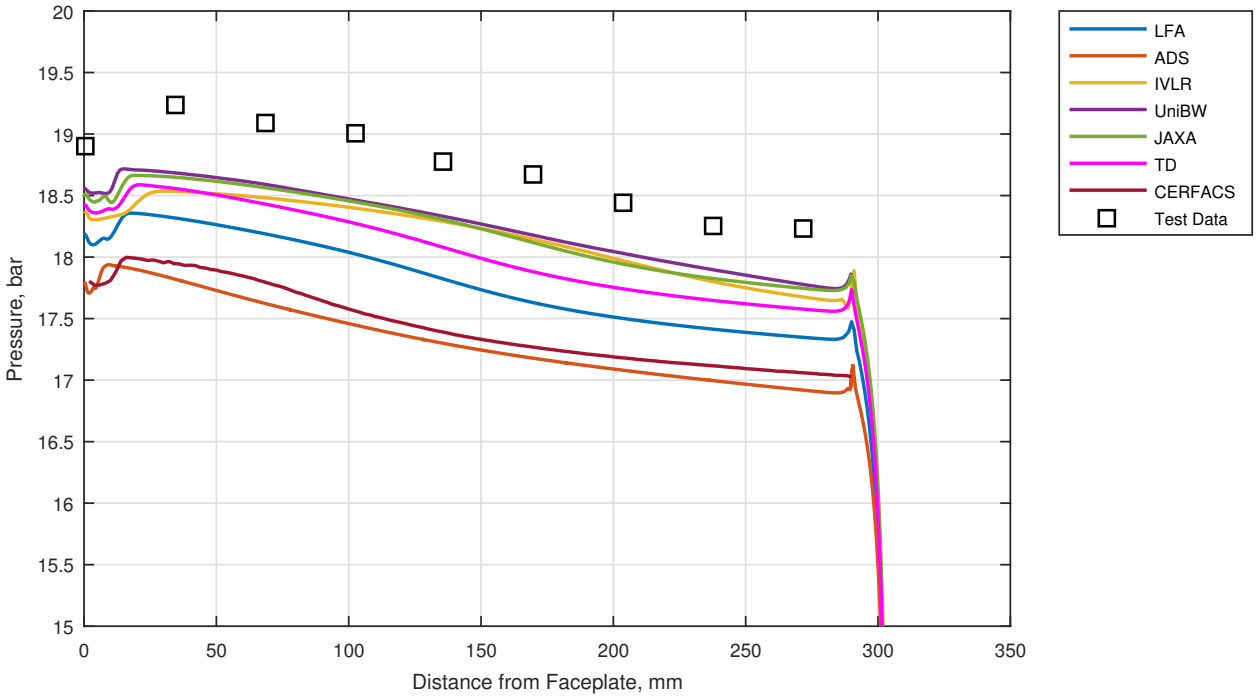

Figure 8: Predicted pressure distribution in the combustor.

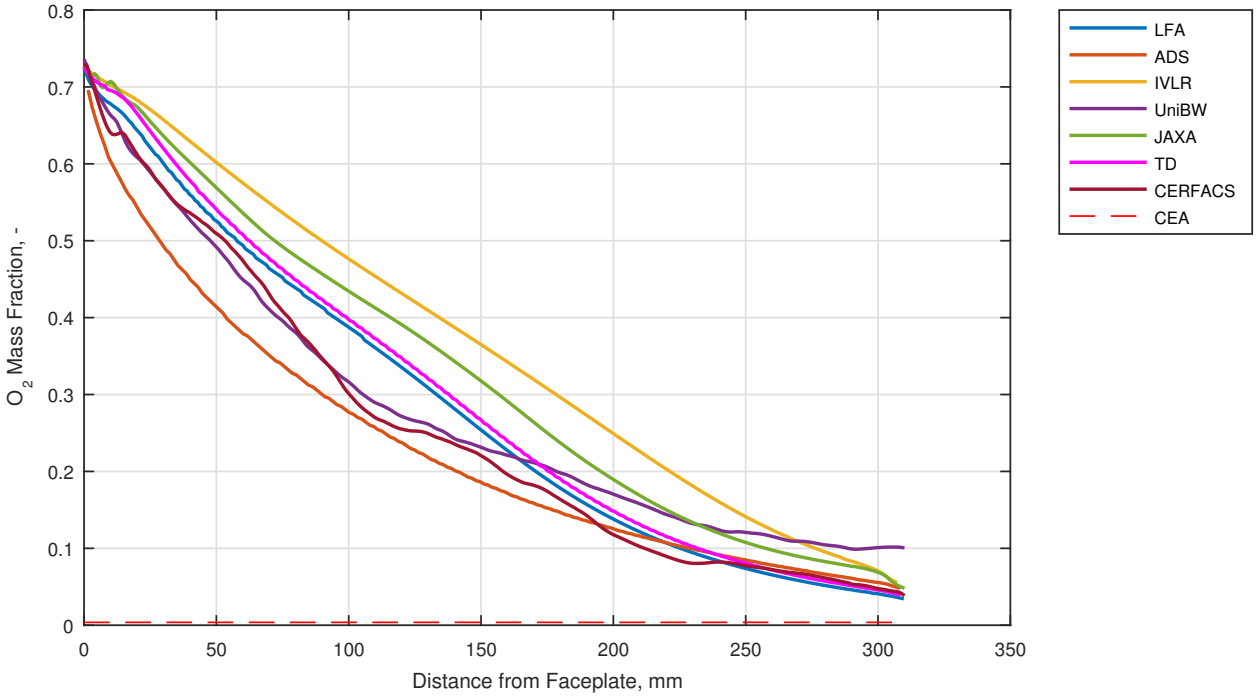

Figure 9: Mass fraction of oxygen mass flow averaged over each cross section along the combustor axis.

the current state the differences between the predictions themselves as well as the differences between the predictions and the experimental data are still considerable. In general it can be said that due to deviations among the computational results more research is required.

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