# Simulation of Single-Injector Methane Rocket Combustor Using Different Numerical Codes

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A single-injector methane combustion chamber is simulated using two different computational fluid dynamic codes: TAU and Fluent, density-based and pressure-based solvers, respectively. The simulated test case is the capacitively-cooled rocket combustor fed with gaseous methane and oxygen and operated at pressure of 19 bar. The aim of the simultaneous simulations is to compare the performance of the two algorithms of solving the Navier–Stokes equations: density-based and pressure-based. Earlier the density-based and pressure-based approaches have not been compared at rocket engine conditions. The simulations were carried out using the same mesh and as much as possible similar setups. Both simulations, TAU and Fluent, agree with each other and with the experimental data well. The Fluent pressure-based solver has showed much faster convergence than the TAU density-based solver due to a larger pseudo-time step and the really two-dimensional setup.

**Key Words:** Computational fluid dynamics, Reactive flows, Rocket combustion chambers, Methane

## 1. Introduction

In spite of the development of the computational fluid dynamics (CFD) in the last two decades, no conventional methods exist for modelling of combustion and heat transfer in rocket combustion chambers. There is an understanding that a proper simulation of a combustion chamber of a liquid rocket engine should be three-dimensional (3D) and should include a structural part: walls and cooling channels.[1)] Such simulations are very complex and require a lot of working and computational time. Therefore, not only the accuracy of numerical model but the performance of CFD code is also important.[2)]

There are many collective works where the numerical models are compared not only with experiment but also with each other.[3–5)] The works in the frameworks of the international Rocket Combustion Modeling workshops and of the summer schools at the Technical University of Munich showed that the comparison with other numerical models is not less important for the development of the numerical methods than the comparison with experiment. However, the past comparisons were carried out in the absence of common methods and methodology, e.i., numerical models used not only different CFD solvers, but geometries, boundary conditions, combustion models, and turbulent models. Therefore, it is very difficult to draw conclusions about the performance of a particular CFD code using the results of the comparisons.

There is also a basic problem related to CFD codes. In rocket combustion chambers, the velocity of gas varies in a wide range from zero to M=1 and higher. It is not yet clear which CFD codes: density-based or pressure-based, are better for the simulation of rocket combustors. In spite of the recent development of CFD methods, pressure-based codes are still better for incompressible flows (M<0.3), and density-based codes are better for compressible flows (M>0.3). The problem of the numerical stiffness in incompressible flows is solvable. In modern density-based codes, it is solved using a preconditioning. However, this procedure is not yet implemented in our in-house code TAU.[6)] Most of pressure-based codes can also accurately simulate compressible flows; however, they may suffer problems with convergence.[7)] Solver convergence depends on the particular case, and the case of rocket combustion chambers is not standard for CFD and requires an accumulation of knowledge.

The idea of the present work is to carry out a proper comparison of solvers of two different CFD codes: the pressure-based Fluent[8)] and the density-based TAU. In order to draw conclusions about the performance of the compared solvers, the comparison is carried out using the same geometry, numerical mesh, boundary conditions, turbulent model, and combustion model.

## 2. Test case

As a test case for the simulations, the TUM test case with a round combustion chamber was chosen.[9,10)] The test case is wall heat flux measurements in a coaxial single-injector combustion chamber fuelled by gaseous methane and oxygen. Methane is the next-generation rocket propellant, for which the combustion is not well characterized yet.[11,12)] Thus, the test case is relevant. The combustion chamber allows simulations in 2D axisymmetric geometry, which is used in the present work. Such simplification reduces significantly the simulation time and does not affect the results of the present work. The previous test case from the same group was a combustion chamber with a square cross-section.[13)] The flow in the square cross-section chamber has a 3D structure.[14)] The different distances from the injector to the side wall results in different sizes of the recirculation zone in the corner of the combustion chamber. The new test case is free from this drawback.

The combustion chamber is shown in Fig. 1. It is a capacitively-cooled rocket combustor with thick copper walls. The combustion chamber is relatively long at a very small inner diameter, see Fig 2. It is designed for low pressures, low mass flow rates, and low heat loads. It is instrumented with thermo-

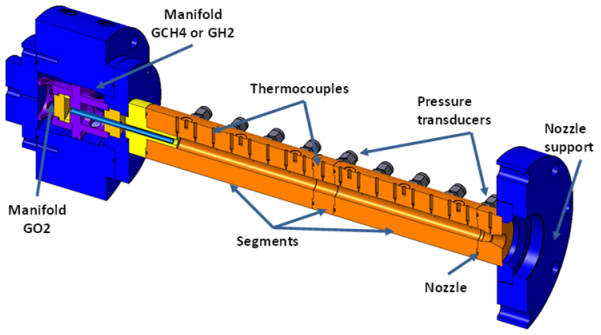


Fig. 1. Single-injector methane sub-scale rocket combustor.[10)]

Table 1. Hot-fire test conditions ($CH_4$, ROF=2.2).[9,16)]

| Items | Values |
|---|---|
| ROF | 2.2 |
| Chamber pressure | ≈19 bar |
| Wall heat flux | max. 8 MW/m$^2$ |
| Injection temperature for $CH_4$ | 268 K |
| Injection temperature for $O_2$ | 276 K |
| Mass flow rate $CH_4$ | 15.3 g/s |
| Mass flow rate $O_2$ | 33.9 g/s |

couples and pressure sensors. The design of the injector and other details of the combustion chamber can be found in original paper.[9)] The targets of simulations are supposed to be a wall heat flux and the pressure in the combustion chamber at the given wall temperature profile .

The hot-fire tests were performed for six load points: three for methane and three for hydrogen. We selected one load point with methane at a ratio oxidizer-to-fuel ROF=2.2 for the simulations that is similar to a previous test case, which was already simulated by us.[15)] The particular test case and load point was already simulated by Daimon et al.[16)] The conditions of the selected hot-fire test are present in Table 1. The main drawback of the test case is a relatively high error of the mass flow rate measurements, which were done on the basis of pressure drop measurements on calibrated orifices. The comparison of two hot-fire tests with the same mass flow rates shows the difference in the chamber pressures of 0.5 bar.[16)] The authors of the test case earlier reported maximum absolute errors of propellants mass flow rates for their test facility.[13)] The values given in the report results in the maximum error of 4% of the total mass flow rate of propellants. This means the uncertainty of 0.8 bar in chamber pressure. The uncertainty in the mass flow rate also leads the uncertainty in wall heat flux; however, the main contributer in the uncertainty of wall heat flux is the uncertainty of the locations of the thermocouples. The accuracy of the heat flux measurements amounts typically to 10–15% in such combustion chambers.

## 3. Numerical setup

The numerical setup is based on our previous simulations with the DLR TAU code.[15)] In the present study, we performed simulations in TAU-code[6)] first and then "imported" the setup into ANSYS Fluent[8)] and repeated the simulations. Both simulations are carried in the same 2D axisymmetric numerical domain and mesh, see Fig. 2.

### 3.1. TAU simulation

The DLR TAU-Code is a finite volume, density-based compressible flow solver for hybrid meshes.[6)] The Favre-averaged Navier–Stokes (FANS) equations are solved employing a Gudonov type finite-volume scheme. For the discretization of the inviscid flux terms an AUSMDV upwind scheme in combination with a MUSCL-type least square algorithm for reconstruction of the second order spatial gradients is used. An explicit 4-th order Runge–Kutta scheme is used for time integration. For convergence acceleration a local time stepping concept and implicit residual smoothing algorithms are applied. The turbulence is modelled using the BSL k-$\omega$ model[17)] because it is available in both codes. Turbulent species diffusion fluxes and enthalpy fluxes are modelled via the turbulent Schmidt and Prandtl numbers with constant values of $Sc_{tr}$=0.7 and $Pr_{tr}$=0.9.

The laminar viscosities for each individual species are spline fitted according to Blottner[18)] based on thermodynamic data obtained from Gurvich tables.[19)] In order to obtain the overall laminar viscosity of the gas mixture the mixing rule of Wilke[20)] is applied. The thermal conductivity of each individual species are computed by an Eucken correction modified by Hirschfelder[21)] and the for the heat conductivity of the gas mixture the mixture rule by Herning and Zipperer[22)] is applied.

The laminar flamelet model offers an immense speed up compared to the full Finite Rate Chemistry model (FRC), especially for simulations with more complex reaction mechanisms (above 10 species and 20 reactions). In contrast to the FRC model, where a transport equation for each species and the chemical source terms are computed directly according to the thermodynamical properties in every cell, the chemistry data in the flamelet model is pre-tabulated and only two additional transport equations for the mixture fraction and the variance of the mixture fraction need to be solved during the CFD simulation. Additional information like species composition and energy source terms are obtained from the flamelet tables. Inside the flamelet model the turbulent flames are considered as a combination of multiple thin, laminar and locally one-dimensional so called "flamelets". The database for the flamelet libraries are multiple one-dimensional flame calculations for varying strain rates to consider the effects of flame stretch and a possible accompanying extinction of the flame. The 1D flame calculations are performed in the so called mixture fraction space, where on one side you have pure oxidizer and on the other side the pure fuel, using the software FlameMaster[23)] and the methane reaction mechanism by Zhukov and Kong.[24)] On the contrary to the speed up of the simulations the flamelet model has several substantial drawbacks. For one thing, the generated flamelet table is only valid at a specific pressure. An assumption, which is valid, can be made for the condition inside rocket combustion chambers. It follows the approach of mixed-and-burned and the combustion process is irreversible. This can lead to a model discrepancy, namely near walls, where due to the cooling of the wall large amounts of energy are extracted from the combustion chamber. As the wall heat flux is one of the most desired results of rocket combustion chamber simulations, the effects along the chamber wall and the validity of the flamelet model there is subject to ongoing investigations.

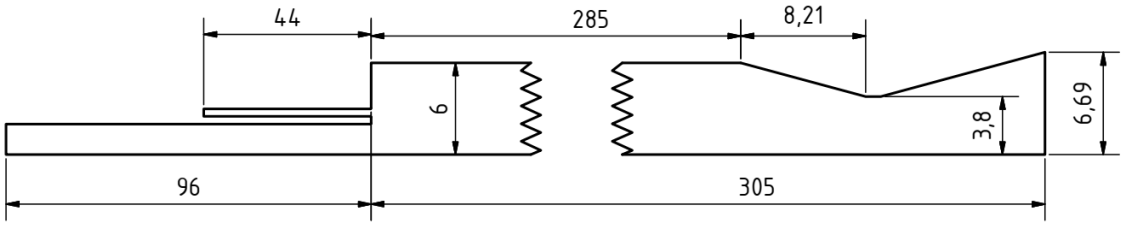


Fig. 2. Sketch of 2D axisymmetric numerical domain.

Table 2. Initial conditions for the CFD simulations.

| Items | Values |
|---|---|
| Pressure | 19 bar |
| Axial velocity | 100 m/s |
| Radial velocity | 1 m/s |
| Turbulent kinetic energy | 500 $m^2/s^2$ |
| Specific dissipation rate | 100 000 $s^{-1}$ |
| Temperature | 1284 K |
| Mean mixture fraction | 0.07 |
| Mixture fraction variance | 0.1 |

### 3.2. Numerical mesh

The numerical mesh was generated using the CENTAUR mesh generator. The mesh includes the oxygen and methane injectors, the combustion chamber, and a nozzle, see Fig. 2. The 2D unstructured mesh has a structured block with a refined mesh in the flame region near the injector and consists of 117 thousand nodes. The mesh also has prism layers near the walls with $y^+$ better than 1. Because there is an influence of spatial discretization on results, this mesh is used the Fluent simulations too.

### 3.3. Fluent simulation

The numerical setup of the Fluent simulation is inherit the setup of the TAU simulations including the mesh. The flamelet library was generated using tools built in Fluent. The mixing rule of Wilke[20] for mixture laminar viscosity was introduced into the model through user-defined functions. The mixture molecular ("laminar") thermal conductivity was calculated from the mixture viscosity using the Prantdl number of 0.7. To solve the Favre-averaged Navier–Stokes equations, the Fluent pressure-based coupled solver was used. According to ANSYS,[25] it is four times faster than the density-based solver in an airfoil simulation at $M$=0.73. The advection term is discretized using the second-order upwind scheme.

To compare CFD solvers in terms of required computational time, both simulations are started from the same initial conditions, see Table 2. The initial conditions are basically an arbitrary uniform field.

## 4. Results and discussion

### 4.1. Results

The results of the numerical simulations are presented in Fig. 3. We can see that results are close to each other. The main visible difference is that the flame is slightly longer in the TAU simulations.

In Figures 4 and 5, the profiles of pressure and wall heat flux are shown. The numerical CFD models agree with each other well. The difference between the TAU and Fluent simulations is insignificant. Probably, the shorter flame in the Fluent simulations results in a higher temperature near the side wall and the higher wall heat flux, and, as a result, in a little bit lower pressure than in the TAU simulations due to higher energy losses.

Both codes also agree with the experimental data well. The experimental data on pressure are shown with error bars of 4%; the data on wall heat flux are shown with error bars of 10%. Both codes predict slightly lower pressure and wall heat flux than the experiment, see Figs. 4 and 5. Both simulations are based on the flamelet model. The classical (adiabatic) flamelet approach predicts slightly lower pressure in rocket combustion chambers.[26] The lower wall heat flux in the simulations has probably the same origin.

### 4.2. Comparison of TAU and Fluent

The TAU and Fluent simulations results are similar, and the difference in the results is insignificant. Both numerical models share the numerical mesh and have the similar advection schemes. The main difference between the TAU and Fluent numerical models is a way of finding pressure and density. From the point of view of a user, the difference between two codes are the computational time and the usability since there is no difference in the simulation results. Therefore, the codes have been compared on these two parameters.

Unfortunately, the used problem formulation did not allow to directly compare the performance of the Fluent and TAU codes. Fluent solved equations on the 2D mesh while TAU solves 3D equations on volume elements. The TAU solver itself creates a 3D mesh of one element thick in the circumferential direction from a 2D mesh. Thus, Fluent and TAU solve different systems of equations in the instant case, and TAU have performs calculations on a twice large amount on nodes. Our Fluent simulation uses the simple model of molecular transport properties. In the TAU simulation, the molecular viscosity and thermal conductivity are modeled more accurately using more calculations. Fluent offers users additional solver settings to speed up the convergence: the control of pseudo-time stepping and of relaxation factors. In the end, the Fluent solver converges to the final solution from the initial conditions, see Table 2, in 772 iterations after several minutes. The process of the convergence of the Fluent solver is shown in Fig. 6. The final TAU simulations took one day on processor Intel Xeon E5-2630 v4 (10 physical cores). There are several low-speed regions in the combustion chamber where the density-based solver needs many iterations to converge. As mentioned above, ANSYS claims that the Fluent pressure-based solver is four times faster than its density-based solver.[25]

With regard to RANS simulations of rocket combustion chambers, it should be noted that computational time and total time spent on simulations are not the same. If the getting of a final solution may require hours, the total time spent on developing of the physical model and the numerical setup, and

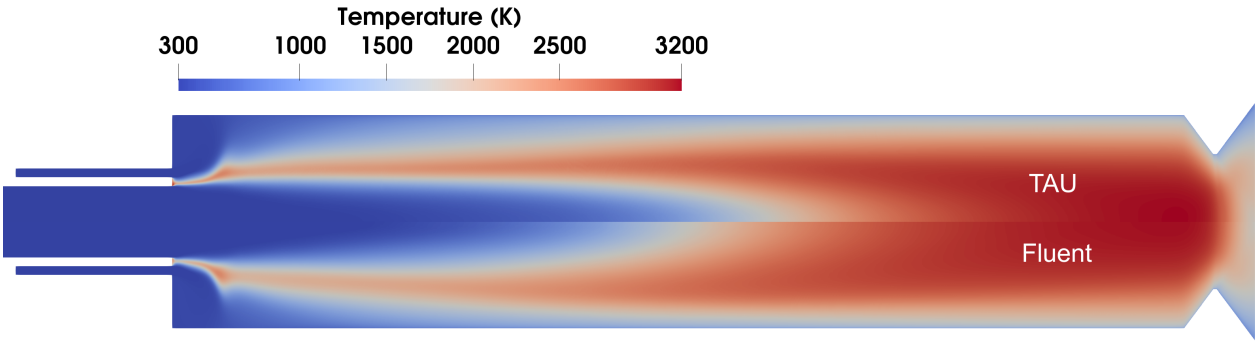


Fig. 3. Simulation results (compressed 5x in the axial direction): TAU (top), Fluent (bottom).

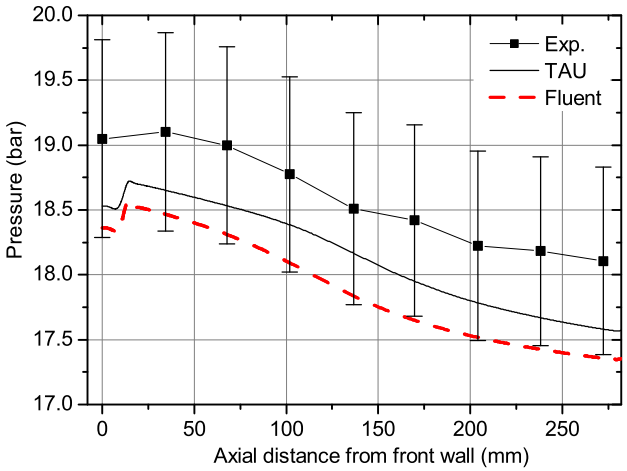


Fig. 4. Wall static pressure profiles: experiment and simulations.

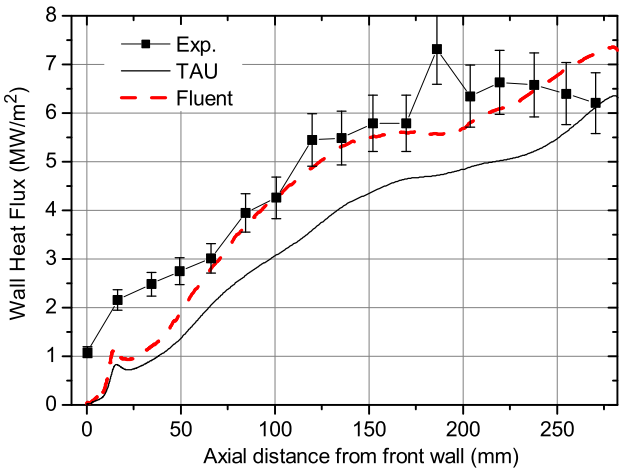


Fig. 5. Wall heat flux profiles: experiment and simulations.

on meshing may take years. In terms of total time spent on simulations, full-featured documentation and convenient mesh generator are not less important than the speed of a solver. The work on CFD simulations is carried out along a converging spiral moving from simple models to complex ones using several tens of numerical meshes. Therefore, the performance of CFD solver is not an ultimate characteristic.

As for the usability, TAU and Fluent are based on different ideologies. Fluent is a mass product with a graphical user interface (GUI), offers a universal tool for any problems. By the way, Fluent gives the choice from three solvers: the coupled pressure-based, the coupled density-based, and a segregated pressure-based solver. Approximately 27% of CFD engineers use Fluent.[27] TAU is, by contrast, an in-house code with a command line interface. In the present study, we are using a customized version developed specifically for rocket applications.[28] Of course, the graphical user interface is the advantage of Fluent while TAU has no GUI and looks outdated. However, the packing of the mesh generator, the pre-processor, the solver, and the post-processor in one interface is not always an advantage. The interface of Fluent is overweighted with buttons and inconvenient. The use of user-defined functions in Fluent required the installation of a third party software, namely, a C compiler.

### 4.3. Comparison with other simulations

The test case was already simulated by Daimon et al.[16] as a case with the recess equal to zero. Daimon et al. performed the simulations in a similar problem formulation also using a 2D axisymmetric domain and solving the FANS equations. Their simulations have a perfect agreement with the experimental data on pressure and a fair agreement on wall heat flux. The flame in the simulations of Daimon et al. is slightly shorter. Daimon et al. simulated reactive flow using a laminar finite rate model with a skeletal reaction mechanism.[16] The finite rate model in contrast of the flamelet model assumes additional heat release in the nozzle which results in a good agreement with the experimental data on pressure.[26,29,30]

## 5. Conclusions

The single-injector combustion chamber fed with gaseous $CH_4$ and $O_2$ has been simulated using the TAU and Fluent solvers, which are density-based and pressure-based solvers, respectively. The simulations have been carried out in the 2D axisymmetric problem formulation by solving the averaged Navier–Stokes equations. The simulations agree with each other well. They also agree with the experiment, but predict slightly lower pressure and wall heat flux. The difference with the experiment is explained by the properties of the used combustion model, namely, the flamelet model.

To compare the TAU and Fluents solvers, both simulations are started from the same initial conditions using the same mesh and as much as possible the same setups. The Fluent pressure-based solver converged in 772 iterations during several minutes. The TAU density-based solver need a day to converge. The Fluent pressure-based solver showed the fantastic speed due to the robust convergence at a large pseudo-time step. Nevertheless, the difference in the numerical setups has not al-

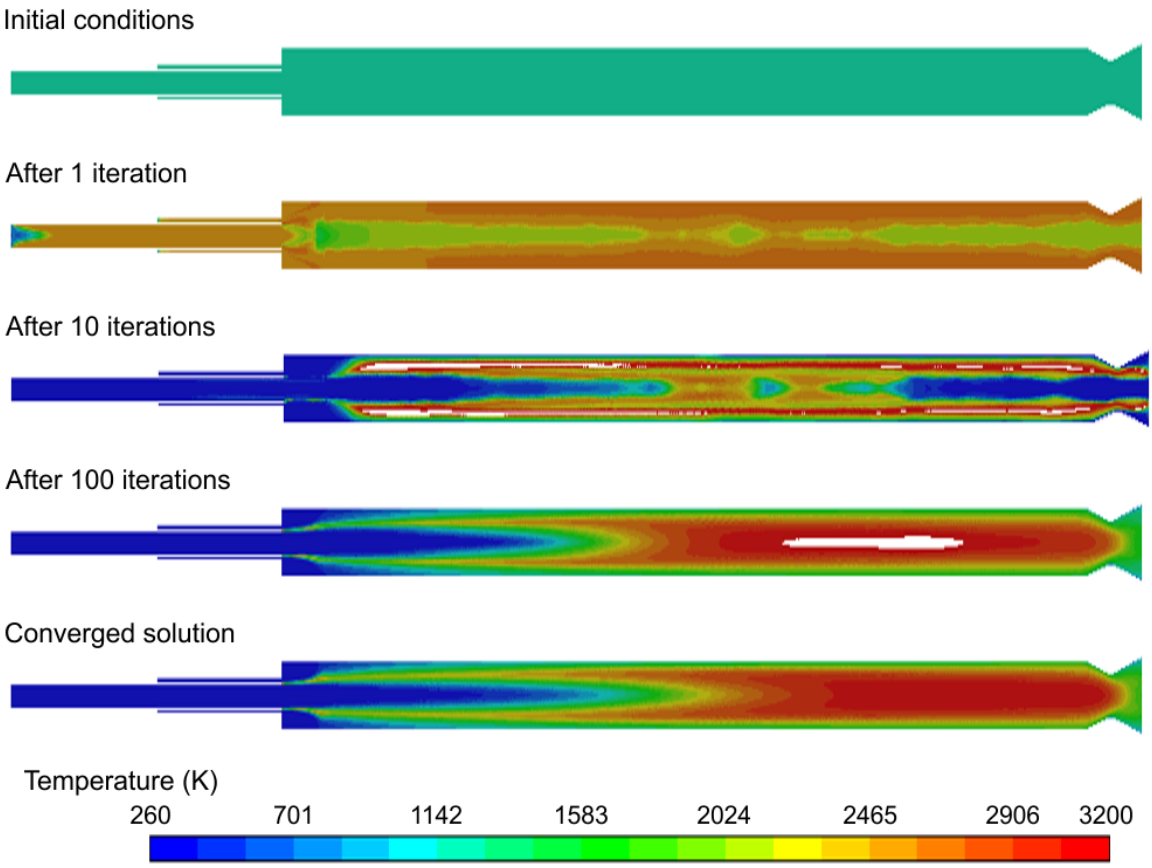


Fig. 6. Temperature field during the convergence of the Fluent pressure-based solver (the image was reflected and stretched twice vertically for better visualization).

lowed the direct comparison of the computational time. In contrast to Fluent, the TAU solver has solved the 3D system of the equations on the double number of nodes.

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## References

1) Eiringhaus, D., Riedmann, H., Knab, O., and Haidn, O. J.: Full-Scale Virtual Thrust Chamber Demonstrators as Numerical Testbeds within SFB-TRR 40, AIAA Paper 2018-4469, 2018.
2) Knab, O., Riedmann, H., Ivancic, B., Höglauer, C., Frey, M., and Aichner, T.: Consequences of modeling demands on numerical rocket thrust chamber flow simulation tools, *Progress in Propulsion Physics*, **11** (2019), pp. 317–346.
3) Tucker, P., Menon, S., Merkle, C., Oefelein, J., and Yang, V.: Validation of high-fidelity CFD simulations for rocket injector design, AIAA Paper 2008-5226, 2008.
4) Ivancic, B., Riedmann, H., Frey, M., Knab, O., Karl, S., and Hannemann, K.: Investigation of different modeling approaches for CFD simulation of high pressure rocket combustors, *Progress in Propulsion Physics*, **8** (2016), pp. 95–116.
5) Roth, C. M., Haidn, O., Riedmann, H., Ivancic, B., Maestro, D., Cuenot, B., et al.: Comparison of different modeling approaches for CFD simulations of a single-element GCH4/GOX rocket combustor, *Sonderforschungsbereich/Transregio 40—Summer Program Report 2015*, 2015, pp. 101–118.
6) Gerhold, T.: *Overview of the Hybrid RANS Code TAU. In: Notes on Numerical Fluid Mechanics and Multidisciplinary Design*, Springer Verlag, 2002, pp. 81–92.
7) Miettinen, A., and Siikonen, T.: Application of pressure-and density-based methods for different flow speeds, *Int. J. Numer. Meth. Fluids*, **79** (2015), pp. 243–267.
8) ANSYS Fluent Theory Guide, Release 15.0, ANSYS, Inc., 2013.
9) Roth, C., Silvestri, S., Perakis, N., and Haidn, O.: Experimental and Numerical Investigation of Flow and Combustion in a Single Element Rocket Combustor using GH2/GOX and GCH4/GOX as Propellants, 31st International Symposium on Space Technology and Science, Matsuyama, Japan, 2017-o-4-01, 2017.
10) Negishi, H., Nakajima, T., Keller, R., and Gerlinger, P. M.: Heat Flux Estimation on a Chamber Wall of GH2/GOx and GCH4/GOx Single Element Rocket Combustors, 31st International Symposium on Space Technology and Science, Matsuyama, Japan, 2017-o-4-02, 2017.
11) Preuss, A., Preclik, D., Mading, C., Gorgen, J., Soller, S., Haidn, O., et al.: LOX/Methane Technology Efforts for Future Liquid Rocket Engines, 5th International Spacecraft Propulsion Conference & 2nd International Symposium on Propulsion for Space Transportation, 2008.
12) Hagemann, G., Onofri, M., Schlechtriem, S., Wilson, F., and Rudnych, M.: Plenary round table: LOX Methane, Space Propulsion 2016, Rome, 2016.
13) Celano, M., Silvestri, S., Schlieben, G., Kirchberger, C. , Knab, O., and Haidn, O.: Transregio SFB-TR40 — Test Case 1. Single Element Combustion Chamber GCH4/GOX, 2015.
14) Keller, R., and Gerlinger, P. M.: Numerical Simulations of a Single Injector Gaseous Methane Rocket Combustion Chamber, AIAA Paper 2016-2148, 2016.
15) van Schyndel, J., Zhukov, V. P., Oschwald, M.: Numerical Simulation of a single-injector GOX/GCH4 combustion chamber using TAU Code with a finite rate chemistry model, Space Propulsion 2018, Seville, Spain, SP2018_00184, 2018.
16) Daimon, Yu, Terashima, H., and Tani, H.: Numerical Investigation

on Effects of Recess Variation upon a GCH4/GOX Shear Coaxial Combustion Chamber, 31st International Symposium on Space Technology and Science, Matsuyama, Japan, 2017-o-4-11, 2017.
17) Menter, F. R., and Rumsey, C. L.: Assessment of Two-Equation Turbulence Models for Transonic Flows, AIAA Paper 94-2343, 1994.
18) Blottner, F. G., Johnson, M., and Ellis, M: Chemically Reacting Viscous Flow Program for Multi-Component Gas Mixtures, Sandia Laboratories, SC-RR-70-754, 1971.
19) Gurvich, L. V.: *Thermodynamic properties of individual substances*, Hemisphere, 1989.
20) Wilke, C.R .: A viscosity equation for gas mixtures, *J. Chem. Phys.*, **18** (1950), pp. 517–519.
21) Hirschfelder, J. O.: Generalization of the Eucken Approximation for the Heat Conductivity of Polyatomic or Chemically Reacting Gas Mixtures. Conference on Thermodynamics and Transport Properties of Fluids, 1957.
22) Herning, F., and Zipperer, L.: Beitrag zur Berechnung der Zähigkeit technischer Gasgemische aus den Zähigkeitswerten der Einzelbestandteile. *Das Gas- und Wasserfach*, **5** (1936), pp. 69–73.
23) Pitsch, H.: FlameMaster, a C++ computer program for 0D combustion and 1D laminar flame calculations, 1998.
24) Zhukov, V.P., and Kong, A.F.: A compact reaction mechanism of methane oxidation at high pressures, *Prog. React. Kinet. Mec.*, **43** (2018), pp. 62–78.
25) Kelecy, F. J., Coupling Momentum and Continuity Increases CFD Robustness, *ANSYS Advantage*, **2** (2008), pp. 49–51.
26) Zhukov, V. P.: Extended Eddy-Dissipation Model for Modeling Hydrogen Rocket Combustors, *Combust. Sci. Technol.*, forthcoming 2019.
27) Comparing CFD Software, https://www.resolvedanalytics.com/theflux/comparing-cfd-software (accessed April 8, 2019).
28) Wagner, B., Schneider, D., Beinke, S., Suslov, D., Génin, C., Hardi, J., et al.: Rocket Propulsion in TAU: An Overview of the DLR ProTAU Project, 7th European Conference for Aeronautics and Space Sciences, Milan, Italy, 2017.
29) Zhukov, V. P., and Suslov, D. I.: Measurements and modelling of wall heat fluxes in rocket combustion chamber with porous injector head, *Aero. Sci. Technol.*, **48** (2016), pp. 67–74.
30) Zhukov, V. P.: The impact of methane oxidation kinetics on a rocket nozzle flow, *Acta Astronaut.*, forthcoming 2019.