Generic Numerical Test Case to Understand Cryogenic Methane Combustion Dynamics

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Abstract. The accurate numerical simulation of high-pressure rocket combustion chambers is a key element for the design of future space transportation vehicles. In recent years investigations focus more and more on methane-based combustion chambers for which many thermodynamic and combustion issues are still unknown. Experimental investigations indicate that we might have to deal with a close interaction of non-ideal equation-of-state effects together with complex kinetic schemes.

On the numerical side the main challenges include the consistent approximation of thermodynamic effects within a broad temperature range from cryogenic injection up to high temperature effects at combustion. Nowadays simple numerical test cases are missing to study and understand the basic effects during the injection and combustion process, especially with methane as propellant. This open question is addressed by the definition of a simple test case for cryogenic methane combustion and its analysis by applying a range of thermodynamic and kinetic models.

Keywords: Rocket combustion · Methane · Non-ideal EOS · Non-ideal mixture effects · Cubic EOS

1 Introduction

The accurate numerical simulation of jet atomization and high-pressure combustion effects at cryogenic temperatures in rocket combustion chambers is a key element for the design of future space transportation vehicles. In the last years the focus of the research was on the development of methane-based rocket engines. In contrast to the well-understood hydrogen-oxygen rocket engines that have been used during the last decades, Lox/Methane imposes additional difficulties on the simulation of the processes within the combustion chamber. For two main reasons the simulation of a methane combustion chamber imposes difficulties at the high-pressure conditions: (1) the relatively complex kinetic mechanisms require the use of tabulated chemistry schemes (2) the close vicinity to the critical conditions for methane and oxygen. Both critical points are located

M. Pini et al. (Eds.): NICFD 2020, ERCOFTAC Series 28, pp. 47–56, 2021.
https://doi.org/10.1007/978-3-030-69306-0_6

around 50 bar and 150 K. Thus, it is unknown whether vapor-liquid-equilibrium effects (VLE) may have to be considered within the thermodynamic description, especially in case for close-critical combustion pressures that are typically present at throttled operating points typical for future engines. These effects were not significant for technical applications of hydrogen-oxygen combustion chambers due to the low critical pressure of hydrogen.

In cryogenic rocket combustion chamber simulations one major challenge is to correctly predict the flow field, the non-linear mixing processes, as well as the combustion of the cryogenic fuels at high-pressure conditions. This requires the estimation of thermal loads onto the combustion chamber walls of future reusable rocket systems by means of validated numerical methods for industrial applications. In the last years effort has been put on the cryogenic mixture modeling for high-pressure hydrogen-oxygen flames. In order to increase the understanding of the physical and thermodynamic effects within methane powered combustion chambers, detailed numerical and experimental investigations are needed. In many cases the simulation of methane-oxygen is still challenging and only few reference test cases are available in the open literature.

One example is the seven injector gaseous combustor of the TU Munich which was considered by many numerical groups around the world (see, e.g. the review paper of Periakis et al. [8]). However, this test case is limited to gaseous fuels and requires the simulation of a full combustion chamber with limited experimental data for comparison. In our present attempt we aim to extend the simple two-dimensional test case introduced by Ruiz et al. [10] as a numerical benchmark for liquid methane-oxygen mixing and combustion processes. In order to keep the geometry simple, a two-dimensional test case focusing on a cut through a coaxial injector is selected. This models the first part of the jet breakup and mixing. It is evident that due to the inherent three-dimensional structure of turbulence this only allows to conduct numerical sensitivity studies and comparisons. Nevertheless, it is a useful test case for code validation as well as case studies due to its simplicity that allows us to use scale resolving methods for detailed comparisons as well.

In the first part of the publication we describe the scope of the research that includes a short summary of the numerical methods used as well as the EOS approximation and the combustion modeling. This is followed by a description of the test case with the first test results. The publication is concluded with a summary and an outlook on further research activities.

2 Scope of Research

In the scope of this research we have a close look at the thermodynamic processes appearing at the cryogenic interface between the cold liquid oxygen jet and the (gaseous) methane jet at supercritical conditions. Similar to the previous investigations in the original test case proposed by Ruiz et al. [10] with hydrogen/oxygen we choose a (constant) combustion chamber pressure of 100 bar, which is located far in the supercritical part to avoid that mixture VLE effects have an influence.

The baseline case will focus on the similarities between the methane-oxygen and hydrogen-oxygen mixing processes. Here combustion kinetics will not be included. For both fuel/oxidizer combinations the fuel is injected as gas while the oxidizer is cryogenic. For the reference case using the combination hydrogen and oxygen, detailed numerical data is available for comparison (see e.g. [7,10]).

In a second step this case will be extended and a chemical kinetics model for high-pressure combustion of methane will be used. One suitable reaction mechanism is the reduced scheme published by Zhukov and Kong [12] that was already used successfully in other rocket chamber applications. This is a first step towards the inclusion of all features of a rocket combustion chamber allowing a detailed comparison of numerical and thermodynamic models. Due to the simple model configuration, parametric studies are feasible.

3 Methodology

For the simulation of cryogenic reacting mixture we are using the DLR flow solver TAU together with suitable EOS mixture models for the cryogenic states. In the following parts we describe shortly the relevant flow solver parts used in this study.

3.1 Compressible Flow Solver TAU

The baseline ideal gas flow solver is the DLR TAU Code for the compressible Navier-Stokes equations with various Reynolds Averaged Navier-Stokes (RANS) and Detached Eddy Simulation (DES) turbulence models. Only a brief overview is given here, detailed descriptions of the ideal-gas flow solver can be found in Hannemann [3], and Karl [5]. TAU is a hybrid grid, finite volume, compressible flow solver. It has been verified for a variety of steady and unsteady flow cases, ranging from sub- to hypersonic Mach numbers.

In recent years the modeling of the flow solver has been extended to cope with cryogenic flows that are e.g. present in rocket combustion chambers (see e.g. in Fechter et al. [1,2]). For these applications the ideal-gas flow solver was extended to cope with cryogenic fluid mixtures based on tabulation as well as direct evaluation of cubic EOS mixture models. The mixture transport properties are chosen in according to the high-pressure Chung model (as described in [9]).

In addition to the cryogenic thermodynamic handling the kinetic modeling was extended to cope with complex schemes based on a cryogenic flamelet model (see Horchler et al. [4]).

3.2 Cryogenic Thermodynamics

To be able to describe the cryogenic mixture effects we apply a cubic EOS mixture model based on a generalized cubic description. Within the cubic EOS formulation the mixture pressure is described by

$$p = \frac{\rho R_u T}{M_w - b\rho} - \frac{a\alpha(T)\rho^2}{(M_w + \delta_1 b\rho)(M_w + \delta_2 b\rho)} \tag{1}$$

using the cubic EOS mixture coefficients $a\alpha(T)$ and b. The EOS parameters δ_1 and δ_2 can be chosen such that the cubic Peng-Robinson or Soave-Redlich-Kwing cubic EOS (see e.g. Kim et al. [6]) are obtained. Corresponding estimation methods for the transport properties are chosen such that they are valid at these high-pressure conditions, see e.g. the mixture viscosity approach of Chung as described in Poling et al. [9].

It is still an open question is whether non-ideal mixture effects close to the critical point region may need to include vapor-liquid equilibrium calculations to be able to numerically reproduce the correct phase informations. First studies on that topic have been done e.g. by Traxinger et al. [11] comparing simulations to simple experiments for a case without chemical kinetics.

3.3 Combustion Modeling Based on the Flamelet Approach

As methane combustion mechanisms typically consist of many reactions, we follow a Flamelet tabulation approach (for general information about the realgas flamelet modeling see Horchler et al. [4]) that is suitable for the application to combustion processes at cryogenic conditions. We solve the modified set of Flamelet equations [6]

$$\begin{aligned} -\rho \frac{\chi}{2} \frac{\partial^2 Y_s}{\partial Z^2} &= \dot{m}_s \\ -\rho \frac{\chi}{2c_p} \left(\frac{\partial^2 h}{\partial Z^2} - \sum_{s=1}^{N_s} h_s \frac{\partial^2 Y_s}{\partial Z^2} \right) &= -\frac{1}{c_p} \sum_s h_s \dot{m}_s \end{aligned} \tag{2}$$

for different values of the scalar dissipation rate χ. The reduced methane reaction mechanism of Zhukov and Kong [12] is used to tabulate the flamelets in mixture fraction space and provided as a flamelet lookup-table to the compressible flow solver.

4 Test Case Definition

This testcase extends the simple test case introduced by Ruiz et al. [10] for cryogenic liquid oxygen and hydrogen to a new application within the methane environment. In the past several studies were conducted on cryogenic mixing effects of hydrogen and oxygen (see e.g. [7,10]) and the original test case was valuable for the validation of numerical tools for cryogenic mixtures in rocket combustion chambers. A sketch of the numerical domain as well as the boundary conditions of the new test case can be found in Fig. 1. For the test case we maintain a oxidizer to fuel ratio of 2.95, a typical value for methane combustion chambers. The methane combustion chamber experiment of the TU Munich (see e.g. Periakis et al. [8]) used a similar oxidizer to fuel ratio.

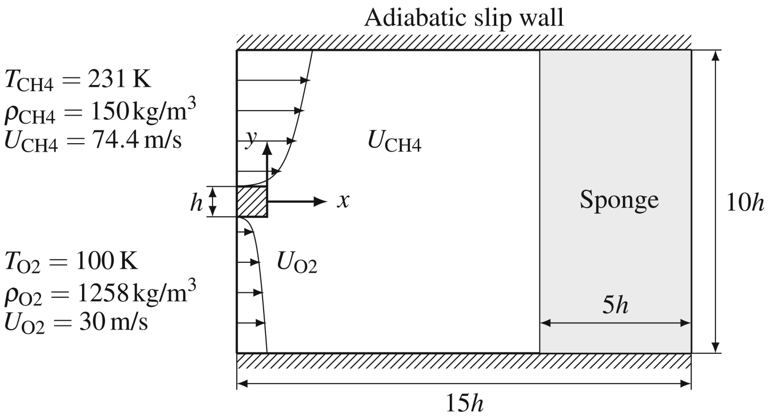


Fig. 1. Sketch of the new mixing test case for Methane/Oxygen following the geometrical definition of the original test case proposed by Ruiz et al. [10].

4.1 New Methane Mixing Test Case

With the increased interest in the modeling of methane, we decided to set up a similar reference test case at conditions typical for methane/oxygen flames at cryogenic conditions. For methane, supercritical conditions are chosen while the oxidizer is injected at a subcritical temperature. At the inlets we impose a $1/7$ power law velocity profile to account for the upstream tubing prior to the injector.

4.2 New Methane Reacting Test Case

As an extension of the mixing test case, we consider the same geometry as in the previous case with an additional combustion model. Due to the large combustion kinetics of methane flames, we apply a realgas flamelet approach. The used kinetics scheme is based on the methane mechanism published by Zhukov and Kong [12] that is suitable for high-pressure methane combustion.

5 First Results

In this paper we include the first results for the Ruiz mixing and reacting test case. A short discussion about the similarities between the original Ruiz test case with fluid pairing hydrogen-oxygen with the proposed new one using methane-oxygen is added.

The authors would like to mention that the direct comparison of RANS and two-dimensional DES/LES solutions is rather quantitative and illustrative. One would expect that a comparison of the two-dimensional RANS solution to a three-dimensional LES simulation would yield different results.

5.1 New Methane Mixing Test Case

In Fig. 2 instantaneous snapshots of the first results of the new mixture test case using the SST turbulence model are shown. A more detailed comparison of the averaged mean values can be found in Figs. 3 and 4. Similar to the outcome of the hydrogen-oxygen Ruiz test case (see e.g. in Fechter et al. [1]), the mean turbulent values can be reasonably well reproduced using a RANS method.

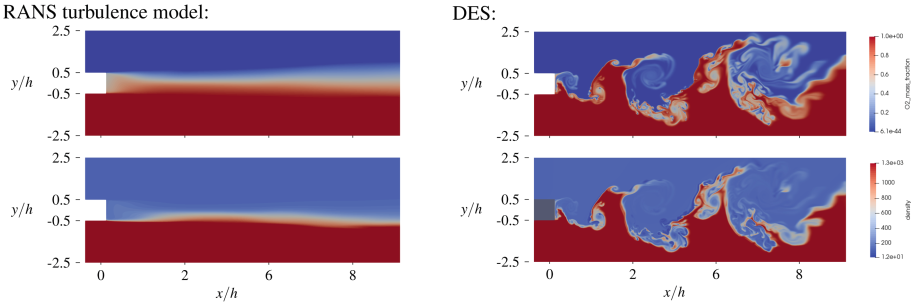


Fig. 2. First results of the new two-dimensional LOX/CH4 mixing case: Left: Averaged fields of oxygen mass fraction and density using the RANS SST turbulence model; Top: Instantaneous snapshots of the oxygen mass fraction and density using a DES turbulence model.

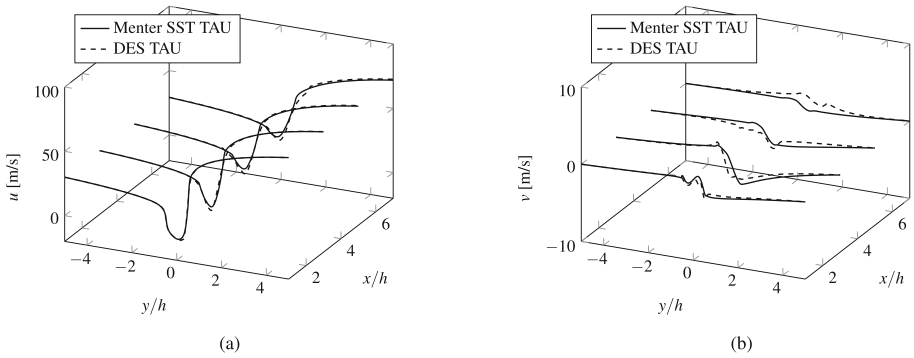


Fig. 3. Transverse cuts of (a) mean axial and (b) mean transverse velocity of the two-dimensional LOX/GCH4 mixing case.

The major differences to the original Ruiz test case [10] using LOX/GH2 is the higher density of the methane at the instream conditions; the oxygen

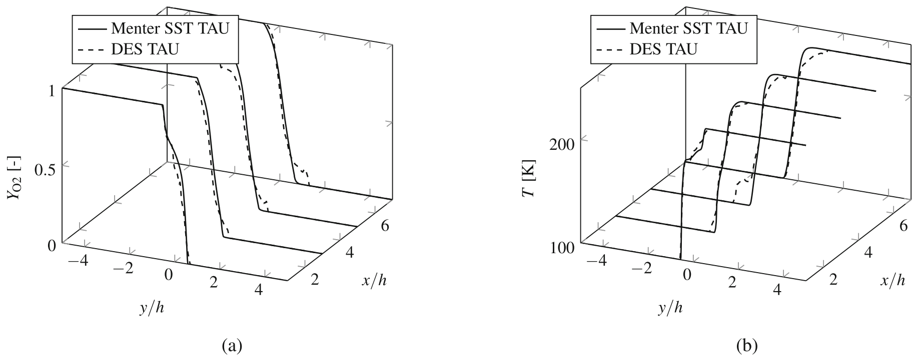


Fig. 4. Transverse cuts of (a) mean oxygen mass fraction and (b) mean temperature of the two-dimensional LOX/GCH4 mixing case.

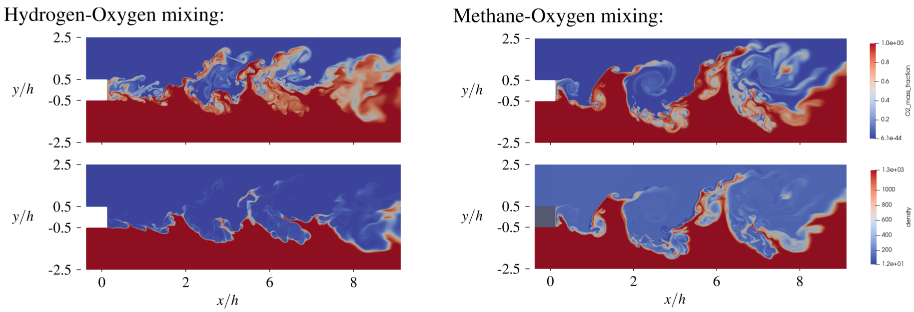


Fig. 5. Comparison of the vortex structures developed in the original Ruiz test case with the fluid pairing hydrogen-oxygen (left) with the new test case for methane-oxygen mixing (right).

conditions are kept unchanged (see comparison of instantaneous snapshots in Fig. 5). Due to the different material properties of the fuel, the Reynolds number for the mixing layer is about twice as large as for the methane case,

$$\mathrm{Re}_{O_2H_2} = \frac{\rho v h}{\nu} = 164 \cdot 10^6 \quad ,$$
$$\mathrm{Re}_{O_2CH_4} = 344 \cdot 10^6 \quad .$$

This increased Reynolds number in the methane test case implies that the small-scale turbulent structuresm that can be identified in the hydrogen-oxygen test case, can not be resolved on the used DES grid. A finer grid would be needed for the methane test case to resolve the same amount of small-scale turbulence structures for the methane mixing test case.

5.2 New Methane Reacting Test Case

In Fig. 6 instantaneous snapshots of the first results of the new reacting test case are shown using the RANS SST turbulence model as well as a DES turbulence

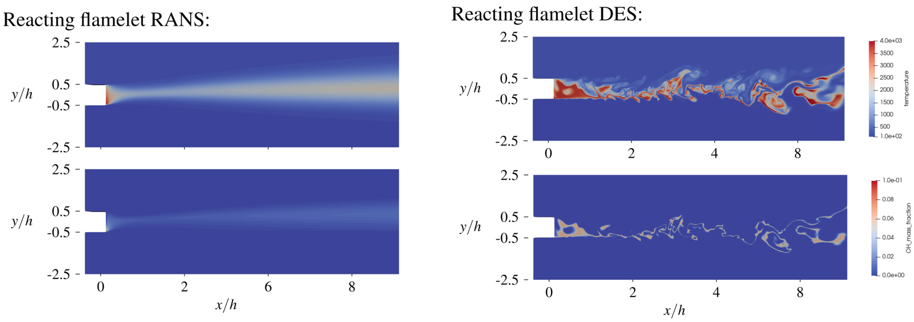
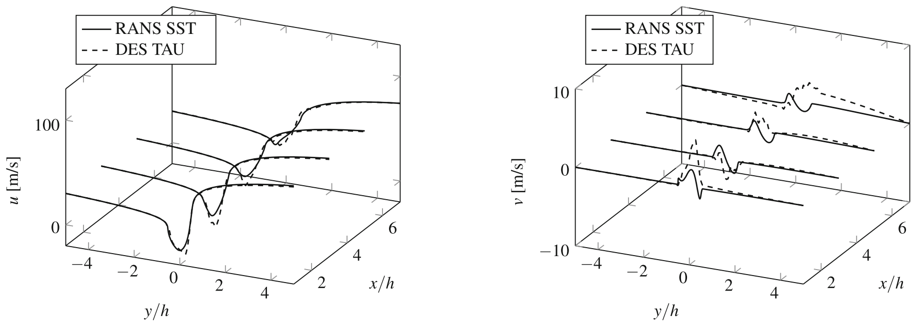
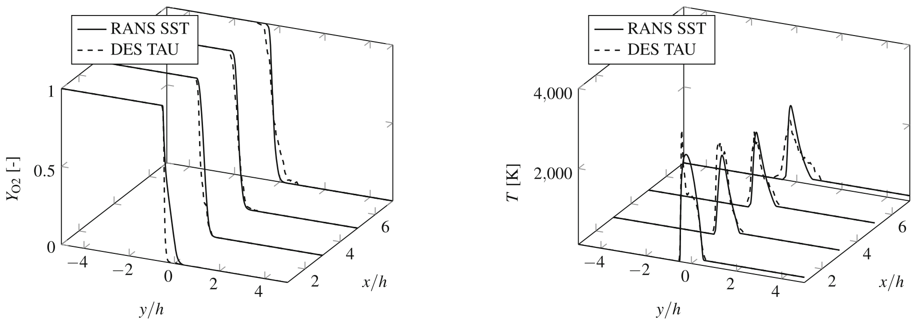


Fig. 6. Comparison of the vortex structures developed in the hydrogen-oxygen reacting test case (left) with the new methane-oxygen reacting test case (right).



(a) (b)

Fig. 7. Transverse cuts of (a) mean axial and (b) mean transverse velocity of the two-dimensional LOX/GCH4 reacting case.



(a) (b)

Fig. 8. Transverse cuts of (a) mean oxygen mass fraction and (b) mean temperature of the two-dimensional LOX/GCH4 reacting case.

model. To model the combustion we apply a Flamelet combustion model with the reduced reaction kinetics described in Zhukov and Kong [12]. The combustion effects are limited to a thin layer inbetween the methane and oxygen streams.

A detailed comparison of the flow features using the averaged mean values can be found in Figs. 7 and 8. Similar to the mixing case, the mean turbulent values can be reasonably well reproduced using the RANS approach. In comparison to the mixing test in Fig. 2 the vortex structures for the reacting case in Fig. 6 are much smaller in size. This is due to the influence of the reactions and the additional temperature gradient in the shear layer.

6 Conclusions and Future Work

We define a generic two-dimensional test case for the mixture and combustion processes of cryogenic methane and oxygen. This simplified two-dimensional numerical test case is inspired by a cut through a coaxial injector and therefore suitable for the validation of numerical methods that aim to describe the physical and thermodynamic effects within the simplified injector geometry. Due to the simplified geometry it is suitable to apply higher scale resolving turbulence modeling approaches like DES or LES in order to tune RANS based turbulence models for this type of applications. This allows us to produce valuable validation data for turbulence models at these cryogenic conditions.

Here we presented the first results for the mixing and reacting test case, comparing the outcome of RANS models to higher resolved DES methods. A first comparison shows a good agreement between the two methods for the mean values. In comparison to the original test case based on hydrogen-oxygen mixing, the methane-oxygen test case shows more turbulent structures in the mixing layer due to the higher Reynolds number and different fluid properties. To resolve these turbulent structures a finer DES mesh resolution is needed. In future this test case might serve as example to investigate the effect of flame anchoring in methane flames.

Acknowledgments. The present work was conducted in the framework of the German Aerospace Center (DLR) project TAUROS (TAU for Rocket Thrust Chamber Simulation) and AMADEUS (Advanced Methods for Reusable Aerospace Vehicle DEsign Using Artificial Intelligence and Interdisciplinary Numerical Simulation) focusing on the qualification and advancement of the DLR flow solver TAU for liquid rocket thrust chamber applications. The financial support of the DLR Space Research Programmatic is highly appreciated.

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