# Modelling of a 7-elements GOX/GCH4 combustion chamber using RANS with EDC combustion model

**By Silong Zhang, Jianfei Wei AND Oskar J. Haidn**

Institute of Advanced Power, Harbin Institute of Technology, No.92 West Da-Zhi Street, 150001, Harbin, China

The report has summarized the computational work conducted by the the group from Harbin Institute of Technology and Prof. Haidn for the SFB-TR40 2017 summer program. A 7-element rocket combustion chamber using GOX/GCH4 as propellant has been modelled and simulated to get a more comprehensive knowledge of the combustion and heat transfer process. All the computational cases in our report used the EDC combustion model for detailed chemistry and two-equations RANS model for turbulence closure. The simulation results show that our model agrees well with experimental data in terms of wall pressure but it overpredicts the heat flux a little in the combustor and underestimate it at the throat. Changing the turbulence model will have great influence on the combustion field and thus the heat transfer conditions. While changing the Prandtl number will change the heat transfer condition without changing the combustion field too much when using RANS model. It has been also found that the reaction mechanism will have great influence on the combustion and heat transfer through having effects on thermophysical properties of the combustion products.

## 1. Introduction

The demanding issues in terms of high operational and handling costs of cryogenic and storable propellants increased the attention for methane/oxygen in the development of future launch vehicles. Methane as a fuel can provide a higher specific impulse, together with better cooling abilities and less soot deposition than kerosene. Differently than oxygen/hydrogen propellant combination, oxygen/methane can be considered as "space storable" and is favored by higher density [1], although it gives lower specific impulse. The adequate understanding and accurate prediction of turbulent combustion, heat transfer characteristics are considered key features for the development of reliable oxygen/methane engines.

Within the frame of SFB TRR40 program, an experimental test campaign was performed at TUM by the group led by Prof. Haidn on a gaseous oxygen (GOX)/gaseous methane (GCH4) shear coaxial 7-elements injector, and wall heat transfer characteristics were discussed. This research aims to build an appropriate CFD model of the 7-Injectors GOX-GCH4 combustion chamber according to the test case provided by Prof. Haidn [2] to help understand the knowledge and details of the combustion process and heat transfer characteristics inside the chamber.

The CFD approach is a very important way to get more details about the flow field inside the combustor and it helps to understand the heat transfer characteristics bet-

ter. To predict the combustion process and heat transfer characteristics accurately in a rocket engine combustor, simplified approaches without the detailed information about the reaction kinetics and thermophysical properties will not work [3, 4].

During the modelling of GOX/CH4 combustion, one of the most important aspects is the choice of the appropriate combustion model: the model should be accurate but also a well compromise between phenomena description and computational costs. A detailed kinetics scheme produces a better description of the flame but a reduced one may produce good results with less time. In the GOX/CH4 combustion processes, the chemical time is typically much smaller than the flow time and correspondingly the Damköhler number(Da) is very large, but the value of Da varies a lot along the combustor length, making locally non-equilibrium reaction near the faceplate of the injectors. Hence it is not possible to assume that the chemistry is infinitely fast all over the combustor. Under these conditions, an Eddy Dissipation Concept model with non-equilibrium reaction considered is more appropriate [5].

For the chemical mechanism used in the model, we will choose two simplified mechanism developed for GOX/CH4 combustion at high pressure. The composite of the combustion products will have significant effects on the heat transfer process through influencing their thermophysical properties both inside and outside the boundary layer [6].

To predict the turbulence appropriately is the key in modelling the combustion and heat transfer process, because the combustion reaction in the rocket engine is mainly controlled by the turbulence and the turbulence is a key factor which determines the heat transfer process in high Reynolds number flow. In this research, two different RANS models for the turbulence were chosen to see their influences on the combustion and heat transfer process.

This work has been carried out in the frame of the SFB/TRR 40 Summer Program 2017. The results are validated against wall pressure and heat flux profiles provided in the test case definition [2]. The basic characters inside the combustor and the effects of turbulent models, turbulence parameters and chemical mechanism on the combustion and heat transfer process will be presented.

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## 2. Reference experiment

The experiment mentioned in this investigation was performed at Technical University of Munich by Simona et al [2]. A 7-elements combustion chamber with circular cross section was used, referring to Ref. [2] for more information about the configuration size and experiment setup. The following is a brief description.

The whole configuration contains seven injectors, combustion chamber and a short nozzle as well as some auxiliary components,as shown in Figure1. The inner diameter and outer diameter of every injector are $4mm$ and $6mm$, respectively. To understand the injector-wall and injector-injector interaction more clearly, all the distances between two injectors and injectors to the wall are identically the half of the injector diameter. The combustion chamber is divided into four sections with the total length of $341mm$ and the diameter of $30mm$. The heat flux of each section were determined by the Calorimetric method. The nozzle is $42mm$ long with a contraction ratio of $2.5$. The scales under concerning are tabulated in Table1.

The experiment was conducted with injecting GOX/GCH4 at $259.4K$ and $237.6K$ respectively. The mass flow rate of oxygen is $0.211kg/s$ and that for methane is $0.080kg/s$.

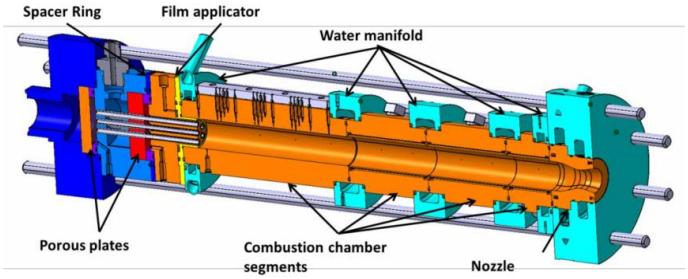



FIGURE 1. Experiment configeration [2].

| | | |
|---|---|---|
| GOX diameter | [mm] | 4 |
| GOX post wall thickness | [mm] | 0.5 |
| GOX post recess | [mm] | 0 |
| GCH4 diameter | [mm] | 6 |
| Injector area ratio $A_{CH4}/A_{GOX}$ | [-] | 0.76875 |

TABLE 1. Injector dimensions.

The exhaust flows out to the ambient atmosphere. All of these will be used as boundary conditions for numerical setup.

A series of thermocouples was placed both in azimuthal and axial direction in order to determine the wall temperature. For comparison between numerical results, the heat flux evaluated by Calorimetric method and the pressure distribution from sensors are both available.

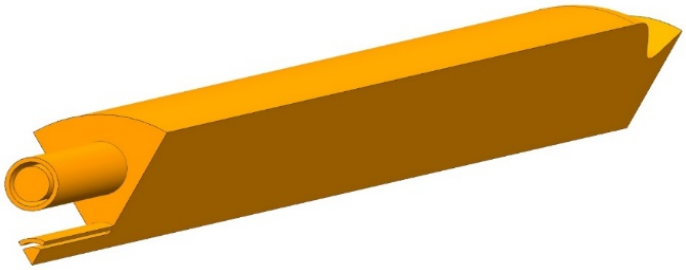
## 3. Numerical method

This section will present the numerical method used in the investigation, including computational model, grids, boundary conditions, turbulence model and turbulence chemistry interaction model for the description of reactive flow. The chemical mechanism and the concerning for thermodynamic properties are also described.

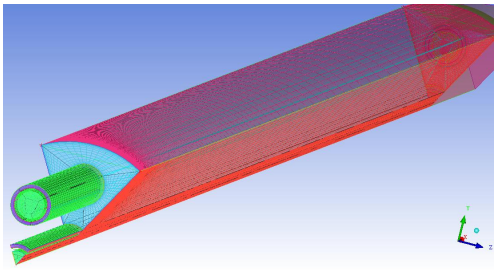
### 3.1. *Physical model and mesh*

For simplicity, only the flow domain is considered, and to improve the computational efficiency, $1/6$ of the flow domain will be taken to build up with grid. To get a fully-developed inlet flow in the combustor, $50mm$ long inlet sections are included for both the methane and oxygen inlets; the other size is set according to the experiment configuration. Figure2(a) illustrates the computation domain.

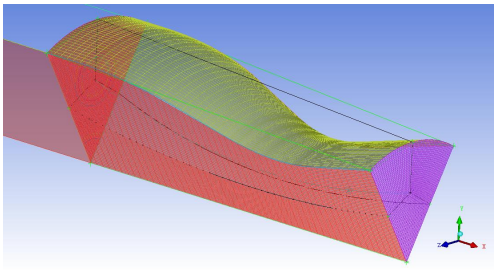
Based on the above physical model, structured grid is used for simulation. In order to simplify the grid generation process, the whole rocket element is divided into two parts, the combustor and nozzle, which can be seen from Figure2(b) and 2(c). Considering the limited computational sources, the total number of the nodes is about $1.3$ million and the wall $y^+$ is kept at almost $1$ at all position. To point it out particularly, the grids near the faceplate are refined in order to get more accurate results for the recirculation zone, which determines the initial mixing of the propellents and thus the combustion process.



(a) The whole model.



(b) Grid generation for the combustor part.



(c) Grid generation for the combustor part.

FIGURE 2. Sketch of computational domain.

### 3.2. *General approach: turbulence and combustion model*

RANS model is used in this report for the turbulence to see its ability to predict the combustion and heat transfer process inside the rocket combustor with GOX and GCH4 as propellents. Standard $k-\varepsilon$ and Realizable $k-\varepsilon$ models were used to see the effects of turbulence model on the prediction results. Since the heat transfer condition is very important here, the enhanced wall treatment is embedded in the turbulence model to solve the region near the wall. The turbulent transport of species and enthalpy are taken into consideration by turbulent Schmit and Prandtl numbers, respectively.

To get a full consideration of the detailed chemistry, reflecting the non-equilibrium reaction process and its effects on the combustion and heat transfer condition, Eddy Dissipation Concept(EDC) model for combustion developed by Magnusson [7] is used.

During the study, two different reduced mechanisms, one from Dong Gang [8] with $14$ species and $18$ reactions, and another one from E.L Petersen [9] with $22$ species and $34$ reactions are presented.

### 3.3. *Boundary conditions and thermodphysical properties*

The boundary conditions are summarized in Table2. The mass flow boundary condition is imposed on the inlet plane according to the experimental data and the pressure outlet condition is applied to the outlet plane with a fixed value, $1bar$. The injector wall and faceplate wall are supposed to be adiabatic and non-slip, while the measured temperature profile is prescribed to the chamber wall as boundary condition. The temperature of the nozzle wall is set artificially to $412K$.

For the thermophysical properties in this report, the thermo database from GRI-MECH 3.0 is used [10], while the density is calculated using ideal gas law. The thermal conductivity and viscosity of propellents and their products are both particularly important to predict the heat transfer process. In this report, the above mentioned two basic thermo-

| Boundary | Type | Specific | Temperature |
|---|---|---|---|
| Injector GOX | Mass flow | 0.211 kg/s | 259.4 K |
| Injector GCH4 | Mass flow | 0.080 kg/s | 237.6 K |
| Outlet | Pressure outlet | 1 bar | - |
| Injector wall and faceplate | Non slip wall | - | Adiabatic |
| Combustor chamber wall | Non slip wall | - | Polynomial fitting |
| Nozzle wall | Non slip wall | - | 412 K |
| Symmetric plane | Symmetry | - | - |

TABLE 2. Boundary conditions for numerical setup.

| | Turbulence model | Pr | Sc | TCI | Chemistry mechanism |
|---|---|---|---|---|---|
| Case 1 | Standard $k-\varepsilon$ | 0.85 | 0.70 | EDC | 14species [8] |
| Case 2 | Standard $k-\varepsilon$ | 0.90 | 0.70 | EDC | 14species [8] |
| Case 3 | Realizable $k-\varepsilon$ | 0.85 | 0.70 | EDC | 14species [8] |
| Case 4 | Standard $k-\varepsilon$ | 0.85 | 0.70 | EDC | 22species [9] |

TABLE 3. Numerical case specifications.

physical properties are calculated by Kinetic theory and ideal gas mixing law methods was used for the mixture.

## 4. Results and Discussion

This section will present the numerical results of difference cases and their comparison to the experimental data. The base case will be discussed in details firstly to describe some important phenomena, and the comparison of heat flux as well as pressure with the experimental data will be conducted. The discussion about the influence of Prandtl number will follows. Last, the concerning will move on to the turbulence model and chemistry mechanism.

Table3 shows all the cases setup in this investigation.

### 4.1. *Analysis of the base case*

The base case in this report refers to Case 1 which is given in Table3.

Figure3 and 4 illustrates the contour of the temperature and the average temperature along the axial direction respectively. The maximum temperature acquired is $3490K$, reasonable to the actual process.

It can be seen from Figure3 that the flame structure anchors at the faceplate and expansion gradually. At the $130mm$ downstream, the combustion is generally completed, which is depicted in Figure4. The whole process of combustion appears to have three different stages, from the initially mixing dominant process to both mixing and kinetically controlled stage, and as the temperature increases, finally present a high temperature chemistry stage controlled by turbulence mixing. Also near the wall of the combustion chamber, an apparent temperature boundary layer can be seen due to the cooling effect. In this region, a relatively low temperature environment slows down the reactions, which need high active energy, therefore, causing the accumulation of water and carbon monoxide as illustrated in Figure 5(a) and 5(b).

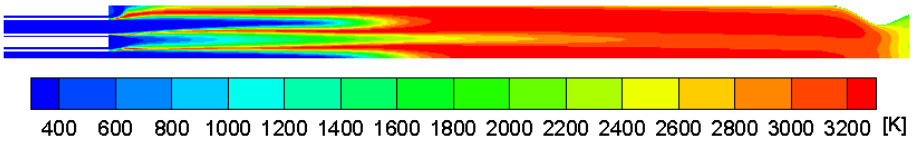



FIGURE 3. Temperature field of the slice at angle 0.

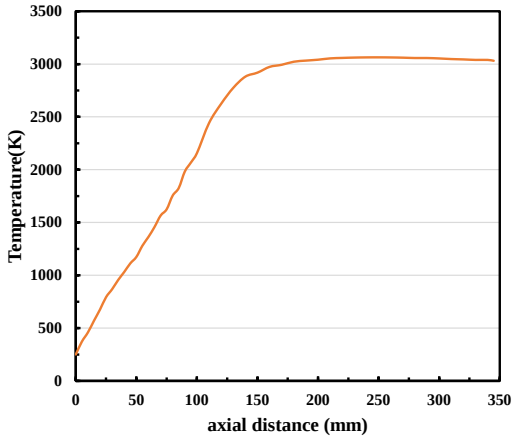



FIGURE 4. Mass weighted average temperature along the combustor length.

Figure 6(a) and 6(b) gives the comparison of the pressure and heat flux between the simulation and experimental data. From the figures, it can be seen that the pressure curve agrees with the experimental data quite well except for little underestimation at the second half part.

While the calculated heat flux is not so satisfactory when compared to the experimental data. The result shows a $2MW/S^2$ overestimation which warns the deficiency of the numerical setup.

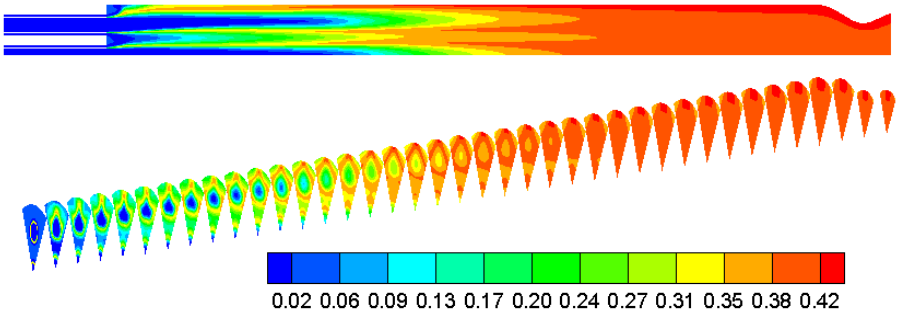
### 4.2. *Effect of Prandtl number*

Turbulence Prandtl number is used to consider the effect of turbulence on the transport of heat, it is defined as a ratio of kinematic viscosity to thermal diffusion coefficient. For RANS simulation used in this report, Prandtl number has negligible influence on the core combustion field, but can change the heat flux through the wall profoundly. Obviously, as the Prandtl number increases, the thermal diffusion coefficient will decrease correspondingly, then, the heat transfer will be weakened, leading to an decreased heat flux and increased pressure, which can be seen from Figure 7(a) and 7(b).

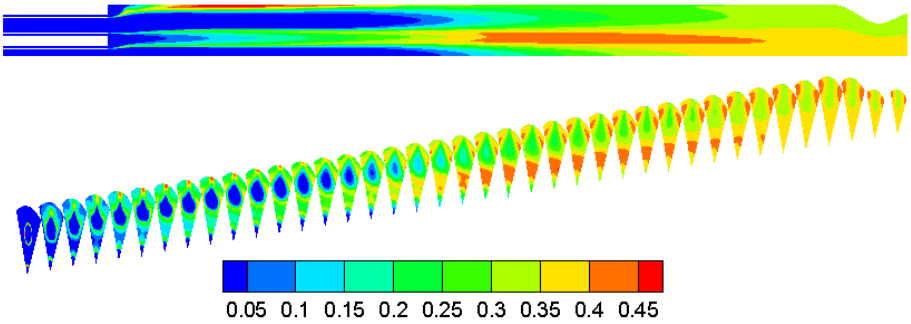
### 4.3. *Effect of turbulence model*

Turbulence has a profound influence on both the flow and combustion. From Figure 8 it can be seen that the flame structure of Realizable $k-\varepsilon$ model is apparently longer than that of Standard $k-\varepsilon$ model, which results from the underestimation of the initial mixing process. For the Realizable $k-\varepsilon$ model, the unburnt gas extends nearly to the nozzle inlet, but this is contrary to the experiment result that imply a complete combustion.

The heat flux and pressure distribution of the two turbulence models are shown in Figure 9(a) and 9(b). It is interesting that the heat flux predicted by the Realizable $k-\varepsilon$

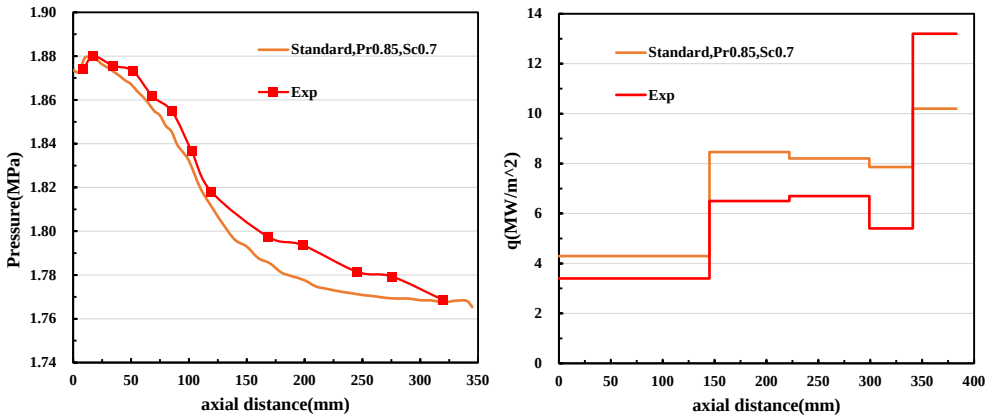



(a) Distribution of $H_2O$ mass fraction along the combustor.




(b) Distribution of $CO$ mass fraction along the combustor.

FIGURE 5. Contours of species distribution

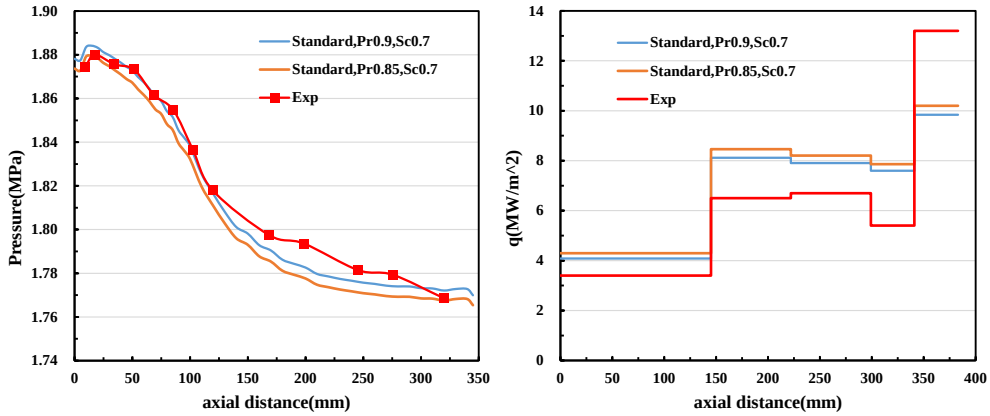



(a) Comparison of pressure between the experimental data and simulation results.

(b) Comparison of heat flux between the experimental data and simulation results.

FIGURE 6. Heat flux and pressure profiles for the experimental data and simulation results.

model is much lower than that of standard $k-\varepsilon$ model and it is much closer to the experimental data. But it should be noted that this phenomenon arises from the poor estimation of mixing process when using realizable k-e model, which is quite contrary to the real situation. This seemingly more accurate result is just coincidentally acquired




(a) Pressure profiles at different Prandtl number.

(b) Wall heat flux profiles at different Prandtl number.

FIGURE 7. Pressure and wall heat flux profiles with PR=0.85 and PR=0.9.

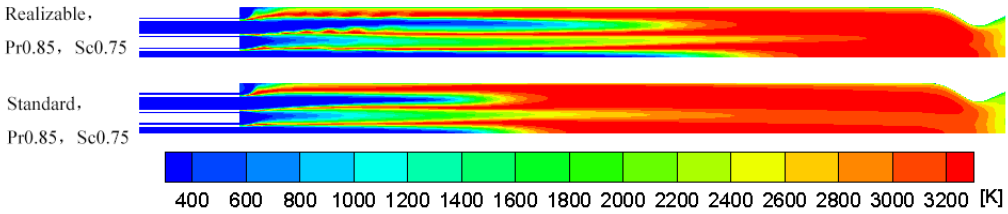
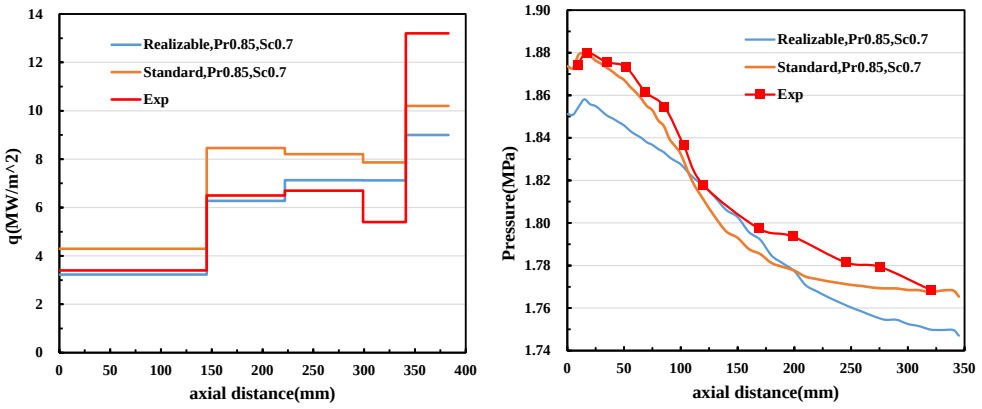



FIGURE 8. Temperature contour for different turbulence model




(a) Heat flux profiles.

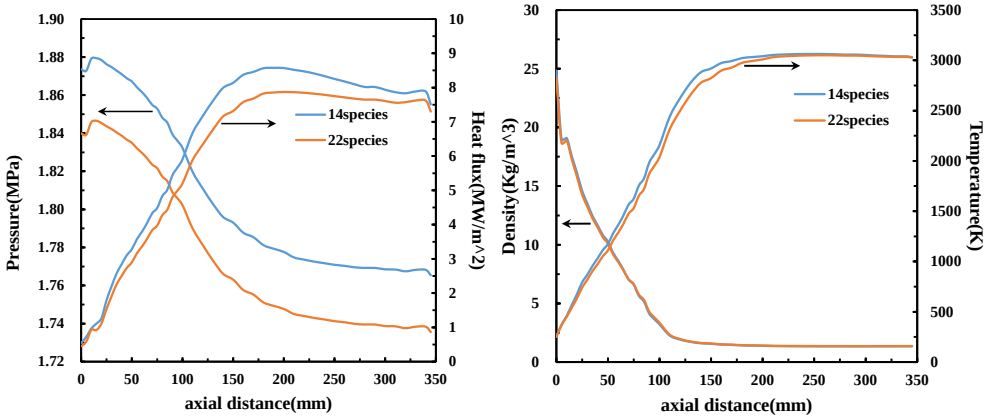
(b) Pressure profiles.

FIGURE 9. Wall heat flux and pressure profiles of the two turbulence model.

due to the delayed combustion, which can be clearly seen from the pressure curve in Figure 9(b).

### 4.4. *Effect of chemical mechanism*

The influence of different chemical mechanism is investigated by the comparison between the results of Case 1 and Case 4.




(a) Pressure and heat flux profiles. (b) Temperature and density profiles.

FIGURE 10. Pressure, wall heat flux, temperature,and density profiles along the axial distance.

From Figure 10(b), it is clearly that both the results show nearly the same temperature and density profiles especially in the second half part of the combustor. However, the pressure profile of Case 4 is lower than that of Case 1 about $0.3Mpa$, it is interesting to note that the two pressure profiles just have the same shape and tendency in Figure 10(a), as if there is a overall pressure decline in the whole combustor. In Figure 10(a),the wall heat flux of Case 4 is also lower than that of Case 1, which is caused by the pressure difference.

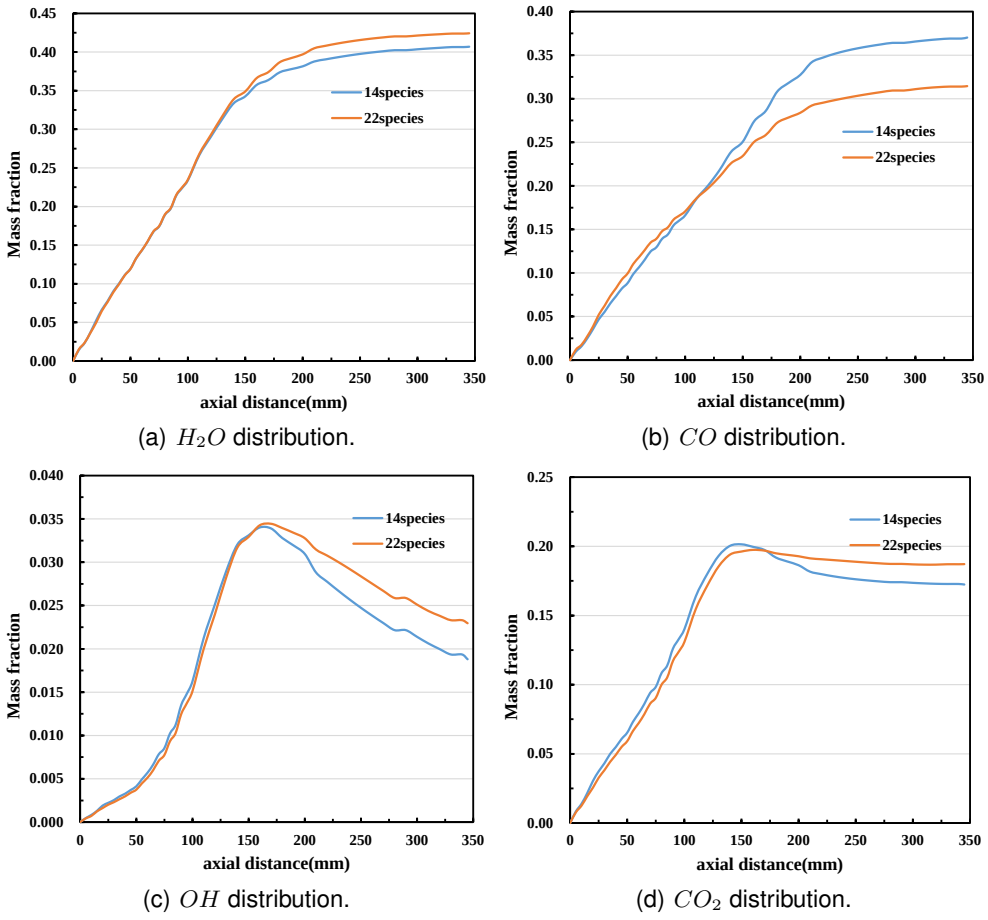
When it comes to the reason for the overall pressure drop, the thermophysical properties of the burnt gas must be considered, especially the specific heat ratio, which is a measurement for the performance of gas expansion.

From Figure 11, different chemistry mechanisms show a different composition of burnt gas especially in the high temperature region. In detail, the mechanism contains $22$ species tends to have more products such as $CO_2$ and $H_2O$, while the mechanism contains $14$ species have more $CO$ contrarily. The difference of the composition will contribute to different thermophysical properties, such as the specific heat ratio shown in Figure 12(a). With the same temperature, density, but different specific heat ratio, the expansion process in nozzle is rather different, as can be seen from the velocity profiles shown in Figure 12(b). The specific heat ratio before expansion process in Case 4 is lower than that in Case 1 at the second half part, which meas a weaker expansion performance as is shown in the velocity profiles. This cause a remarkable decline of pressure in the combustion chamber, and then, leading to a distinct heat flux distribution.

## 5. Conclusions

A 7-element rocket combustion chamber using GOX/GCH4 as propellant has been modeled and simulated, the results have been discussed comprehensively in four aspects: the basic case and phenomenon, the effect of Pr number, the effect of turbulence model, and the effect of chemical mechanism.

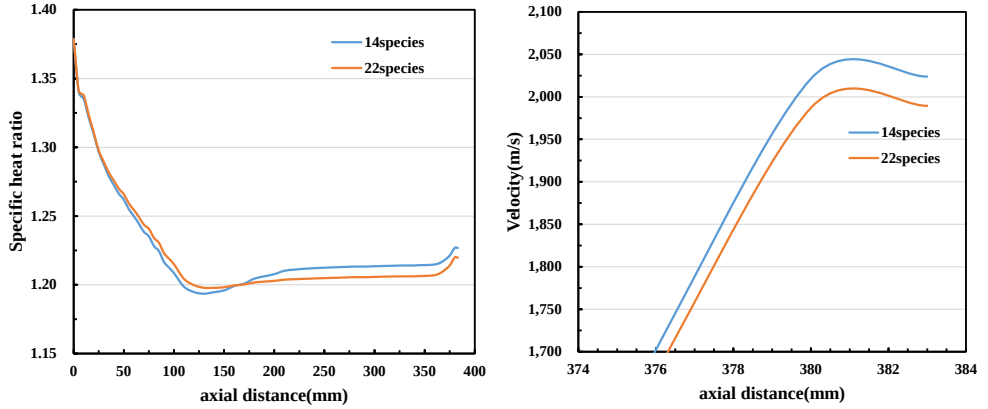
The computational results show that the RANS methods coupled with EDC model can capture the main characteristics of the combustion process in the GOX/GCH4 combustion chamber equipped with seven injectors. The pressure profiles predicted by the simulation are rather accurate when compared to the experiment data. Three different




(a) $H_2O$ distribution. (b) $CO$ distribution.

(c) $OH$ distribution. (d) $CO_2$ distribution.

FIGURE 11. Species distributions along the axial distance.




(a) Specific heat ratio profiles. (b) Nozzle velocity profiles.

FIGURE 12. Profiles for specific heat ratio and velocity discrepancy.

stages discussed in the base case are found in the whole combustion process, these stages imply some inequilibrum chemistry which is the starting point of using EDC combustion model. The EDC combustion model has the advantage of incorporating the influence of finite rate kinetics at computational cost using a reduced chemical mechanism, and the turbulence-chemistry interactions are taken into account by reference to the phenomenological description of turbulence in terms of the turbulent energy cascade.However, none of the presented simulation results shows a satisfactory agreement with the experiment data on the heat flux aspect, the heat flux of the combustor part is overestimated, and that of the nozzle part is just the opposite, be underestimated. The possible reason for this deviation could be the combined effect of both flow and turbulence chemistry interaction.

The results also show that some model parameters such as Pr number only influence the wall heat flux level when using the RANS method, as to other field variables, the effect could be neglected. For a better prediction of heat flux along the combustor, there demands a thorough investigation on the optimum values for these parameters.

This investigation reveal that the thermophysical properties have significance impact on the whole combustion process. It is well known that thermophysical properties are dominated by the chemical mechanism. In the simulation, different chemical mechanism gives different species composition, and then, changes the thermophysical properties of the burnt gas. The results show different expansion process caused by the discrepancy of the specific heat ratio, and that will contribute to the different pressure level in the combustor. Efforts are needed to find a proper mechanism or to develop other new chemical mechanisms in order to get a more suitable one under the experiment conditions.

The subsequent work will focus on improving the agreement between predictions and experiment data. This may include a deep investigation into the reactive flow process, such as a more thorough comprehension of 3D characteristics, and turbulence-chemistry interactions. For the purpose of improving the flow field predictions, DES, which takes advantages of both the LES and RANS, is under consideration. Besides, the model parameters in both turbulence model and combustion model should be optimized in order to reproduce the real combustion process more accurately.

## Acknowledgments

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## References

[1] PREUSS, A., PRECLIK, D.AND MADING, C. AND GORGEN, J. (2008). Lox/methane technology efforts for future liquid rocket engines. In: *5th International Spacecraft Propulsion Conference and 2nd International Symposium on Propulsion for Space Transportation*.

[2] SILVESTRI, S., CELANO, M.P. AND ROTH, C. (2017). Transregio sfb-tr40-test case bks-2.

[3] IERARDO, N., CONGIUNTI, A., AND BRUNO, C. (2004). Mixing and combustion in supercritical o2/ch4 liquid rocket injectors. In: *42nd AIAA Aerospace Sciences Meeting and Exhibit.* Reno, NV,.

[4] CUTRONE, L., IHME, M. AND HERRMANN, M. (2006). Modeling of high-pressure mixing and combustion in liquid rocket injectors. In: *Proceedings of the Summer Program of the SFBTRR40*.

[5] ZONG, N., RIBERT, G. AND YANG, V. (2008). A flamelet approach for modeling of liquid oxygen (lox)/methane flames at supercritical pressures. *AIAA paper*, **946**, 2008.

[6] BERGMAN, T.L. AND INCROPERA, F.P. (Eds.) (2011). *Fundamentals of heat and mass transfer*. John Wiley & Sons.

[7] MAGNUSSEN, B.F. AND HJERTAGER, B.W. (1981). On the structure of turbulence and a generalized eddy dissipation concept for chemical reaction in turbulent flow. In: *19th AIAA aerospace meeting*. St. Louis, USA.

[8] DONG, G., HUANG, Y. AND LIANG CHEN, Y. (2000). Study of effects of different chemical reaction mechanisms on computation results for methane jet turbulence diffusion flame. *Journal of Fuel Chemistry and Technology*, **28**, 49–54.

[9] PETERSEN, E.L. AND HANSON, R.K. (1999). Reduced kinetics mechanisms for ram accelerator combustion. *Journal of Propulsion and Power*, **15**, 591–600.

[10] FRENKLACH M, BOWMAN T, S.G. (2011). Gri-mech 3.0. `http://www.me.berkeley.edu/gri_mech/`. [Online; accessed 2012-03-10].