Warsaw University of Technology

FACULTY OF
POWER AND AERONAUTICAL ENGINEERING

Division of Aircraft Engines

in the field of study Aerospace Engineering
and specialisation Aircraft Propulsion

CFD Analysis of Oxyacetylene Ablation Testing of Thermal Insulation Materials

Cezary Chmielewski
student record book number 292809

thesis supervisor
Phd. Mateusz Żbikowski

Warsaw, 2022

Abstract

The project was the Combustion processes computational simulations course main task. An acetylene torch numerical simulation has been chosen as main subject. Mentioned tool has a wide range of uses in technic and one of than is a heat source during an ablation test. In the time of experiments, materials strength on heat flux are checked. Hot combustion gases are directed along the normal to the specimen until burn-through is achieved. The erosion rate of the material is determined by dividing the original thickness by the time to burn-through. The insulating effectiveness is determined from back-face temperature measurements. Insulation index numbers are computed by dividing the times for temperature changes of 80, 180, and 380°C, from the initial ambient temperature, by the original thickness. The insulationto-density performance is computed. An acetylene torch is one of a test bench integral component, adequately to Standard Test Method for Oxyacetylene Ablation Testing of Thermal Insulation Materials E285-08 [1]. Thus, it was decided to carry on numerous CFD simulation with usage of the open-source code. As the main tool for numerical analysis the OpenFOAM has been chosen. Code enables to create calculation domain, prepare mesh, and include necessary dictionaries to create a solver. This work base on generally available use-case prepared for methane burner. It was noticed that main dictionaries used by the authors has been blockMesh, and reactingFoam. Based on that, domain has been changed and the acetylene was used as fuel. Final results include flame solution and flow around heat flux meter added to the domain.

Keywords: OpenFOAM, CFD, combustion, acetylene torch, ablation test

Contents

List of Figures

List of Tables

Introduction

The project aimed for expand students' lore about numerical simulation of a combustion process. This exercise enables to develop knowledge about specified phenomena and develop skills in numerical calculations. CFD analysis require patient and inquisitiveness, but from the other hand, enable to achieve many more accurate parameter values with lowered costs than experiments carried on dedicated test benches. At the beginning each student had to choose a subject. Thus, it was decided to simulate combustion process in an oxyacetylene torch. Work has been started from research of globally available use-cases with usage of OpenFOAM as the tool for numerical calculations. The OpenFOAM code which is an open-source program enabling to solve flows through a control are and fluid structure interaction. As a result, it returns fluid and solid thermodynamics parameters. An ablation test has been chosen as reference due to interest of possibilities arising from the CFD analysis which can improve the future experiments.

Theory

Acetylene torches Figure 1 are used during oxy-fuel welding and oxy-fuel cutting which are processes that use fuel gases (or liquid fuels such as gasoline or petrol, diesel, bio diesel, kerosene etc.) and oxygen to weld or cut metals. Pure oxygen, instead of air, is used to increase the flame temperature to allow localized melting of the workpiece material (e.g., steel) in a room environment. A common acetylene/oxygen flame burns at about 3,773 K (3,500°C; 6,332°F).

In oxy-fuel welding, a welding torch is used to weld metals. Welding metal results when two pieces are heated to a temperature that produces a shared pool of molten metal. The molten pool is generally supplied with additional metal called filler. Filler material selection depends upon the metals to be welded.

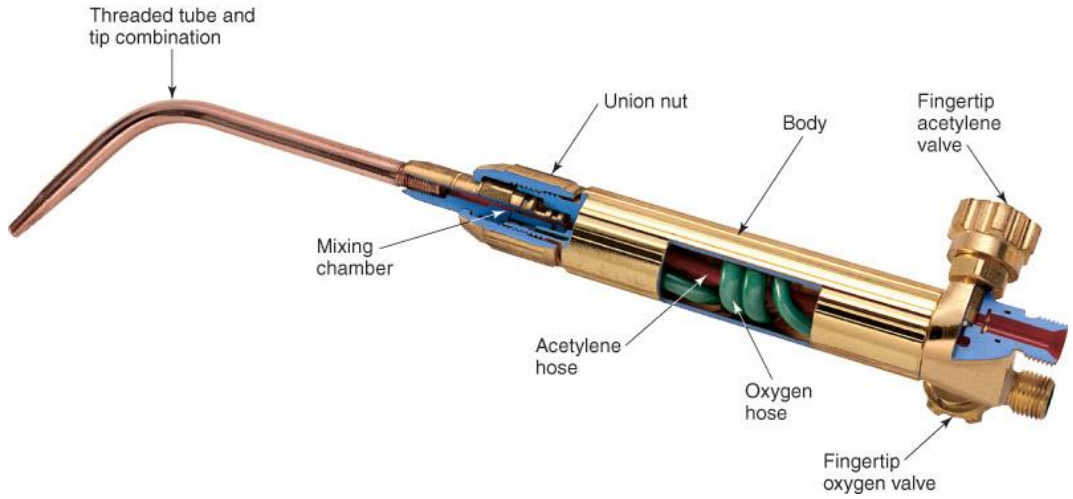


Figure 1 Acetylene torch

In oxy-fuel cutting, a torch is used to heat metal to its kindling temperature. A stream of oxygen is then trained on the metal, burning it into a metal oxide that flows out of the kerf as dross.

Torches that do not mix fuel with oxygen (combining, instead, atmospheric air) are not considered oxy-fuel torches and can typically be identified by a single tank (oxy-fuel cutting requires two isolated supplies, fuel, and oxygen). Most metals cannot be melted with a single-tank torch. Consequently, single-tank torches are typically suitable for soldering and brazing but not for welding.

Acetylene torch purpose:

- Heating metal: in automotive and other industries for the purposes of loosening seized fasteners.
- Neutral flame is used for joining and cutting of all ferrous and non-ferrous metals except brass.
- Depositing metal to build up a surface, as in hardfacing.
- Also, oxy-hydrogen flames are used:
  - in stone working for "flaming" where the stone is heated and a top layer crackles and breaks. A steel circular brush is attached to an angle grinder and used to remove the first layer leaving behind a bumpy surface similar to hammered bronze.
  - in the glass industry for "fire polishing".
  - in jewelry production for "water welding" using a water torch (an oxyhydrogen torch whose gas supply is generated immediately by electrolysis of water).
  - in automotive repair, removing a seized bolt.
  - formerly, to heat lumps of quicklime to obtain a bright white light called limelight, in theatres or optical lanterns.
  - formerly, in platinum works, as platinum is fusible only in the oxyhydrogen flame and in an electric furnace.

In short, oxy-fuel equipment is quite versatile, not only because it is preferred for some sorts of iron or steel welding but also because it lends itself to brazing, braze-welding, metal heating (for annealing or tempering, bending or forming), rust, or scale removal, the loosening of corroded nuts and bolts, and is a ubiquitous means of cutting ferrous metals.

Acetylene torch kit

Regulator

The regulator ensures that pressure of the gas from the tanks matches the required pressure in the hose. The flow rate is then adjusted by the operator using needle valves on the torch. Accurate flow control with a needle valve relies on a constant inlet pressure.

Gas hoses

The hoses are designed for use in welding and cutting metal. A double-hose or twinned design can be used, meaning that the oxygen and fuel hoses are joined. If separate hoses are used, they should be clipped together at intervals approximately 3 feet (1 m) apart, although that is not recommended for cutting applications, because beads of molten metal given off by the process can become lodged between the hoses where they are held together, and burn through, releasing the pressurized gas inside, which in the case of fuel gas usually ignites.

Non-return valve

Acetylene has explosive nature, although it has an upper flammability limit in air of 81%, acetylene's explosive decomposition behavior makes this irrelevant. If a detonation wave enters the acetylene tank, the tank will be blown apart by the decomposition. Ordinary check valves that normally prevent backflow cannot stop a detonation wave because they are not capable of closing before the wave passes around the gate. For that reason, a flashback arrestor is needed. It is designed to operate before the detonation wave makes it from the hose side to the supply side.

Check valve

A check valve lets gas flow in one direction only.

Torch

The torch is the tool that the welder holds and manipulates to make the weld. It has a connection and valve for the fuel gas and a connection and valve for the oxygen, a handle for the welder to grasp, and a mixing chamber (set at an angle) where the fuel gas and oxygen mix, with a tip where the flame forms. Two basic types of torches are positive pressure type and low pressure or injector type.

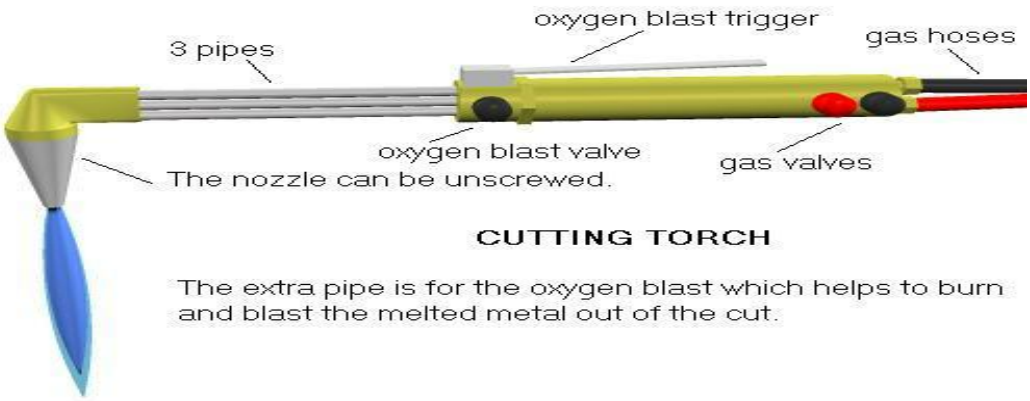


Figure 2 Cutting torch

It can be identified by having only one or two pipes running to the nozzle, no oxygen-blast trigger, and two valve knobs at the bottom of the handle letting the operator adjust the oxygen and fuel flow respectively.

A cutting torch head is used to cut materials. It is similar to a welding torch but can be identified by the oxygen blast trigger or lever.

Acetylene

Acetylene is the primary fuel for oxy-fuel welding and is the fuel of choice for repair work and general cutting and welding. Acetylene gas is shipped in special cylinders designed to keep the gas dissolved. The cylinders are packed with porous materials (e.g., kapok fibre, diatomaceous earth), then filled to around 50% capacity with acetone, as acetylene is soluble in acetone. This method is necessary because above 207 kPa (absolute pressure) acetylene is unstable and may explode.

There is about 1700 kPa pressure in the tank when full. Acetylene when combined with oxygen burns at 3200°C to 3500°C, highest among commonly used gaseous fuels. As a fuel acetylene's primary disadvantage, in comparison to other fuels, is high cost.

Ablation testing

Oxy-acetylene Test Bed (OTB) described in ASTM E285 is a device capable of simulating hyperthermal environments with a heat flux up to 1,000 W/cm^2. Capability of producing reduced, neutral, and an oxidized flame environment. Capability to acquire the in-depth temperature profiles, surface temperature, and evaluate the ablation rate, mass loss, and the post burning morphology of the ablative sample. OTB is usually equipped with ablation recession and thermal sensing technology, capable of measuring recession rate and in-depth temperature using ultra-fine thermocouples from 4- to 9-levels for low density to high density ablators (e.g., 0.20 to 1.8 g/cm^3). A char strength sensor capable of measuring both compressive and shear strength of charred ablatives.

Figure 3 Ablation testing

Stoichiometry

Simplified combustion process can be written via stoichiometry. It assumes that there is one equation for exchange reaction. Its correct for completely combustion when reagents pairs have contact with each other and enough time to find in equilibrium state. However, in real combustion process it is unlikely and before final products establish, sub species create. It is also connected with high particles energy which increase influence of thermal decomposition. Thus, single-step global acetylene-oxygen reaction can be written as:

$$2C_2H_2 + 5O_2 \rightarrow 4CO_2 + 2H_2O + Heat.$$

The single-step reaction mechanism can be extended with more products as:

$$C_2H_2 + \frac{5}{2}O_2 = \sum_{i=1}^{i=n} \omega_i X_i.$$

where:

X_i – the species (CO, CO2, H, H2, H2O, O, O2, OH);

ω_i –the species coefficients.

A more detailed mechanism for the combustion of the most common hydrocarbons has been reported and validated. In particular, it includes the first reaction between the hydrocarbon and the oxygen to produce CO and H2, which in the general case for n-paraffin can be written in the form:

$$C_nH_{2m} + \frac{n}{2}O_2 = nCO + mH_2;$$

This global reaction will be combined with 21 elementary reactions involving the H2 −O2 − CO mechanism. This additional mechanism consists of 12 species. The reactions and rate parameters for the H2 − O2 − CO mechanism is given in Table 1.

Table 1 Reaction mechanism used in quasi-global mechanism for CO−H2−O2 system

Reactions	A	n	Ea
H + O2 = O + OH	2.2 × E14	0	16.8
H2 + O = H + OH	1.8 × E10	1	8.9
O + H2O = OH + OH	6.8 × E13	0	18.4
OH + H2 = H + H2O	2.2 × E13	0	5.1
H + O2 + M = HO2 + M	1.5 × E15	0	-1.0
O + HO2 = O2 + OH	5.0 × E13	0	1.0
H + HO2 = OH + OH	2.5 × E14	0	1.9
H + HO2 = H2 + O2	2.5 × E13	0	0.7
OH + HO2 = H2O + O2	5.0 × E13	0	1.0
HO2 + HO2 = H2O2 + O2	1.0 × E13	0	1.0
H2O2 + M = OH + OH + M	1.2 × E17	0	45.5
HO2 + H2 = H2O2 + H	7.3 × E11	0	18.7
H2O2 + OH = H2O + HO2	1.0 × E13	0	1.8
CO + OH = CO2 + H	1.5 × E7	1.3	-0.8
CO + O2 = CO2 + O	3.1 × E11	0	37.6
CO + O + M = CO2 + M	5.9 × E15	0	4.1
CO + HO2 = CO2 + OH	1.5 × E14	0	23.7
OH + M = O + H + M	8.0 × E19	-1	103.7
O2 + M = O + O + M	5.1 × E15	0	115.0
H2 + M = H + H + M	2.2 × E14	0	96.0
H2O + M = H + OH + M	2.2 × E16	0	105.0

In the H2 − O2 − CO mechanism, there are third-body (M) reactions of two species A and B to yield one single product species AB∗.

$$A + B = AB*.$$
$$AB* = A + B.$$
$$AB* + M = AB + M*.$$
$$M = M* + \text{heat}.$$

The third body M is an inert molecule (in the atmosphere, generally N2 and O2) that can remove the excess energy from AB* and eventually dissipate it as heat.

The H2 − O2 − CO mechanism will provide accurate values for flame characterization. Because the accuracy of the combustion simulations depends primarily on burned gas properties included in the system. In this regard, the more species/reaction will provide more accurate results. However, the computational time should not be skipped. The computational costs of a given reaction are proportional to N2, where N is the number species. The acetylene-oxygen reaction with H2 − O2 − CO mechanism includes 12 species (C2H2, O2, H, O,H2,OH, H2O,N2, CO, CO2, HO2 and H2O2). Hence, the multi-step reaction model used in this study is computationally expensive than other reaction models explained earlier.

CFD simulations

Use-case

For CFD analysis it was necessary to provide required environment. Investigated use-case is dedicated for OpenFOAM 7 and OpenFoam v1912. To run this version of OpenFOAM a hypervisor has been used. The hypervisor VirtualBox enable to put a virtual machine which makes possible to install any operating system independent on nominal placed on used PC. It means that there was possible to install Linux Ubuntu 20.04 LTS which draw from different computer sources than installed OS. The use-case described in [5] has been chosen after research. In this case, authors conduct via simulation of methane burner. Guideless and file sources prepared by the authors have been used. It, enabled to expend possessed knowledge on open-source programs and simulating combustion process with usage of them. Based on source files, first calculations have been carried on compare solution correctness. It required to install in Linux OS, OpenFOAM 7 apart from the newest version.

Proposed model, include methane air combustion inside a burner with applied the system's chemical properties defined by GRI 3.0. Combustion the model Eddy Dissipation Concept (EDC) has been included. The EDC model is based on Eddy Dissipation Model. This model splits the fluid into reacting zones (called "fine structures") and non-reacting zones (called "surroundings"). Fine structures are the regions where the dissipation of turbulence energy takes place. Fine structures have a tube-like shape with the diameter at the order of Kolmogorov's length-scale.

In use-case, the Sandia D Flame burner has been analyzed. Authors prepared simplified geometry which is presented on Figure 2.1.

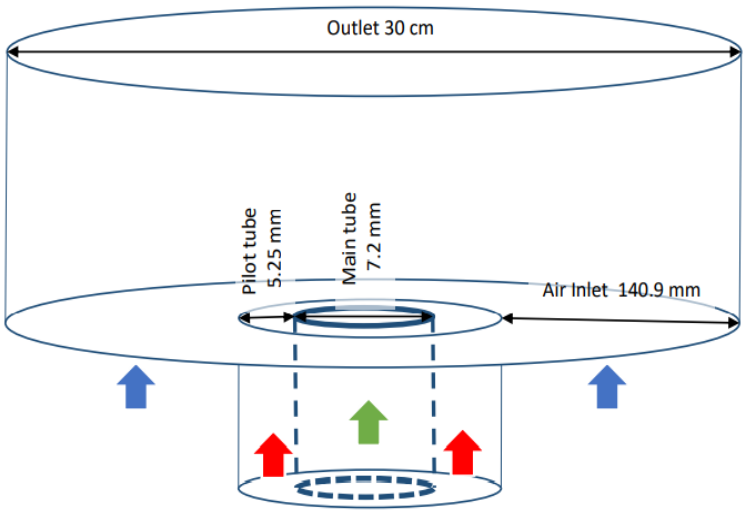


Figure 4 Use case geometry

To sum up boundary conditions, Table 2 has been prepared. Noteworthy is that three inlets have been applied in the model. From symmetry axis, through main jet flow fuel with air, pilot jet delivers pre combusted mixture of CH4 and air. Surrounding has been imitated via additional air inlet which deliver clean air.

Table 2 Boundary conditions

		Streams		
		Main Jet	Pilot Jet	Air Flow
Temperature		294	1880	291
Velocity		49.6	11.4	0.9
Mass Compositions	CH4	0.1561	0	0
	O2	0.1996	0.054	0.23
	CO2	0	0.1098	0
	H2O	0	0.0942	0
	N2	0.6473	0.7342	0.77

Mesh

For numerical calculations, 5^{o} axisymmetric part of domain presented on Figure 5 has been created. Boundary conditions has been applied the same as presented on figure above and additionally periodic condition has been added on side surfaces created via cross section.

Figure 5 Control domain

In next step, whole domain has been divided on finite elements. The blockMesh dictionary was used as tool for preparing calculation domain. It requires additional text file where mentioned

dictionary is applied. The text file consists rare points of geometry coordinates, blocks division and information about the boundary conditions. During the blocks setting, mesh size and refinement have to be defined. Figure 6 presents preview of created mesh.

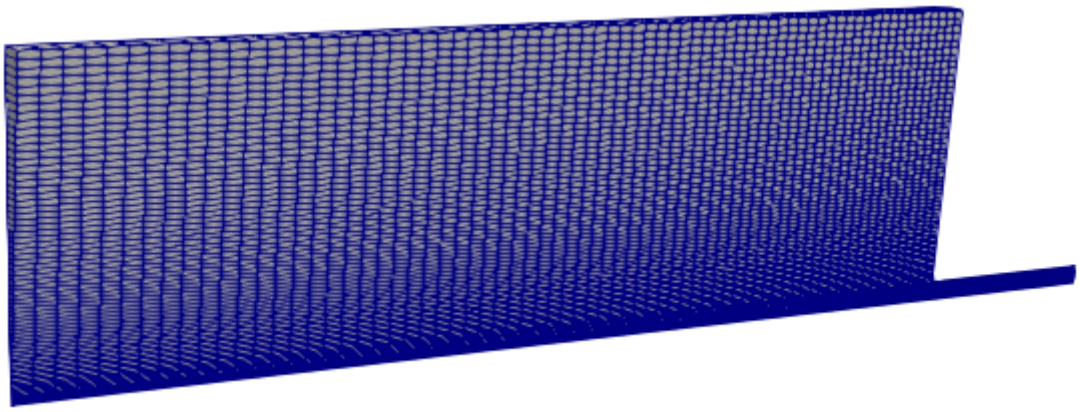


Figure 6 Mesh

Additional mesh refinement along axis has been included via simpleGrading feature. Mesh resolution has been increased in the most important region. Figure 7 presents scope for refinement effect observed near inlets area.

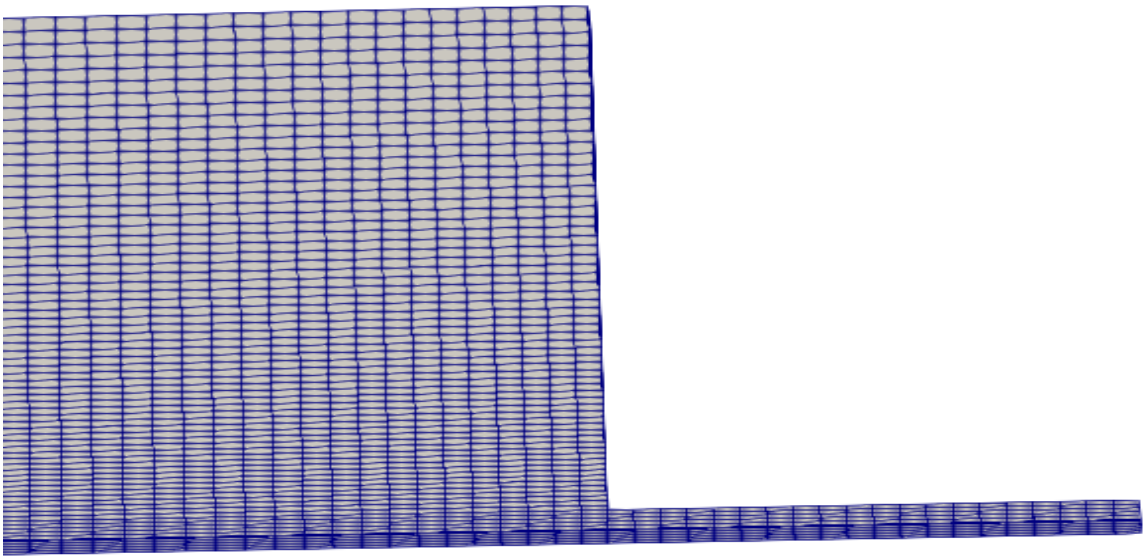
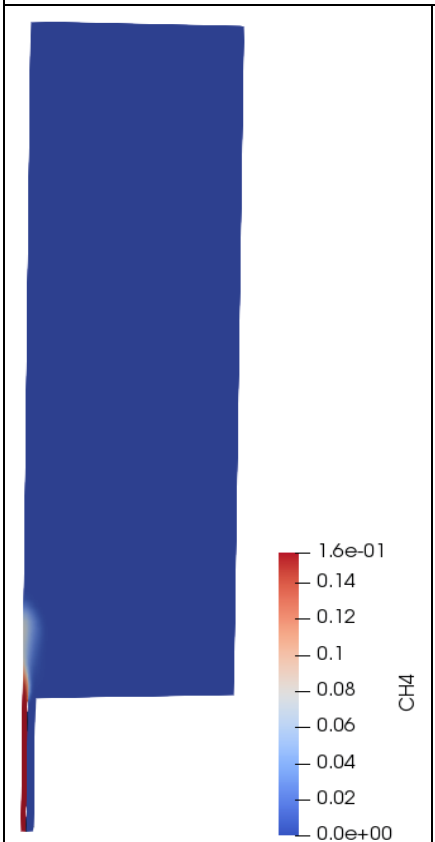
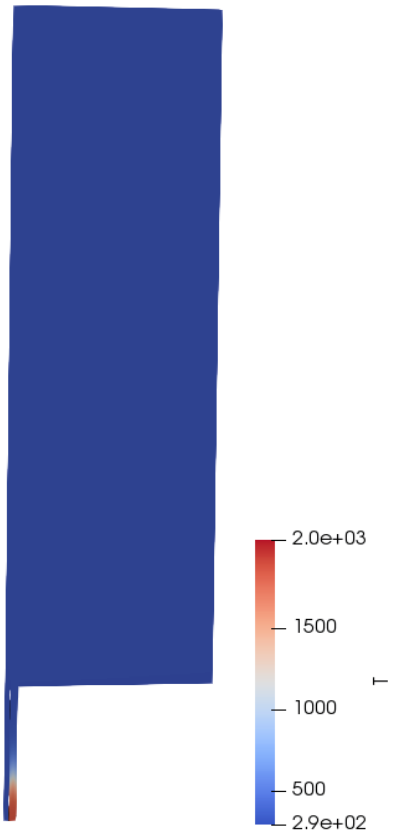
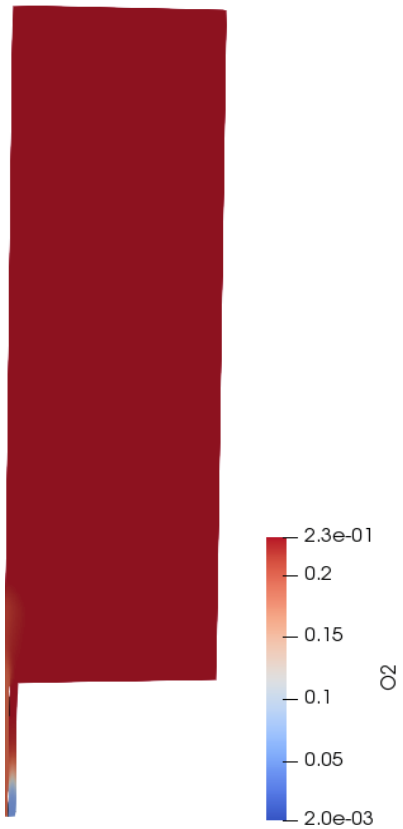
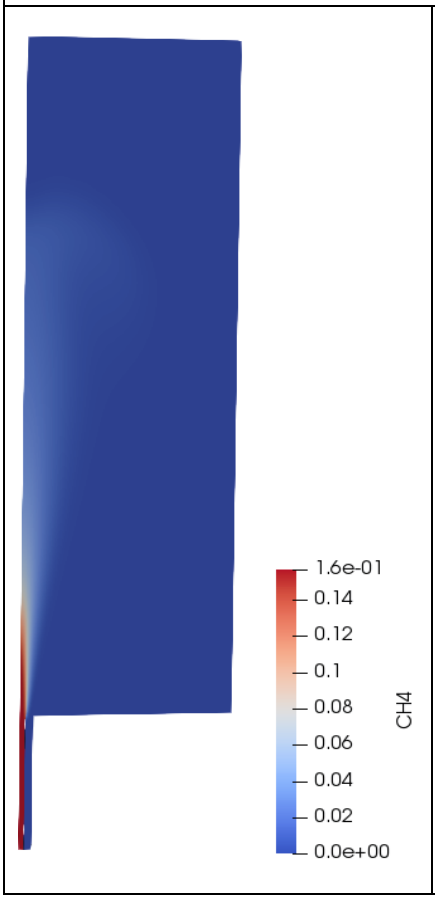
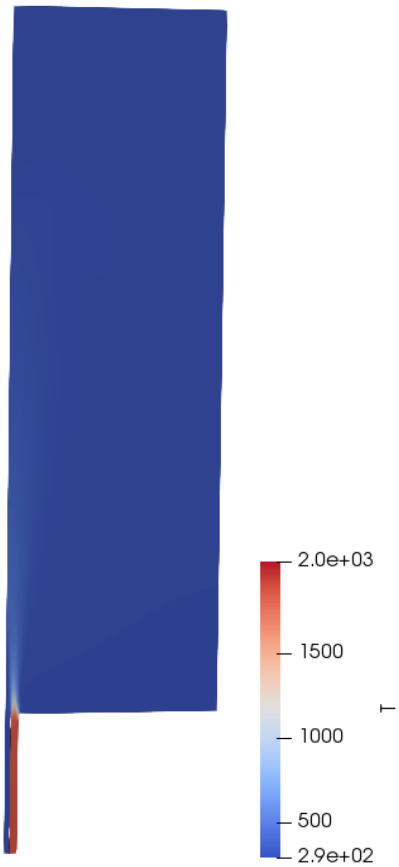
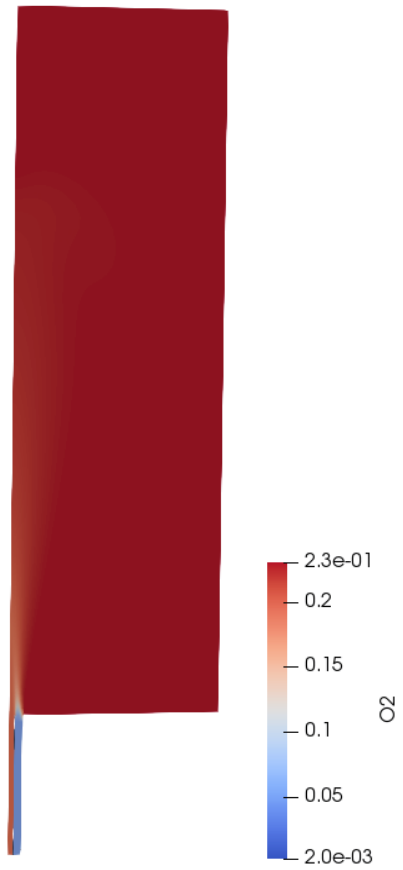


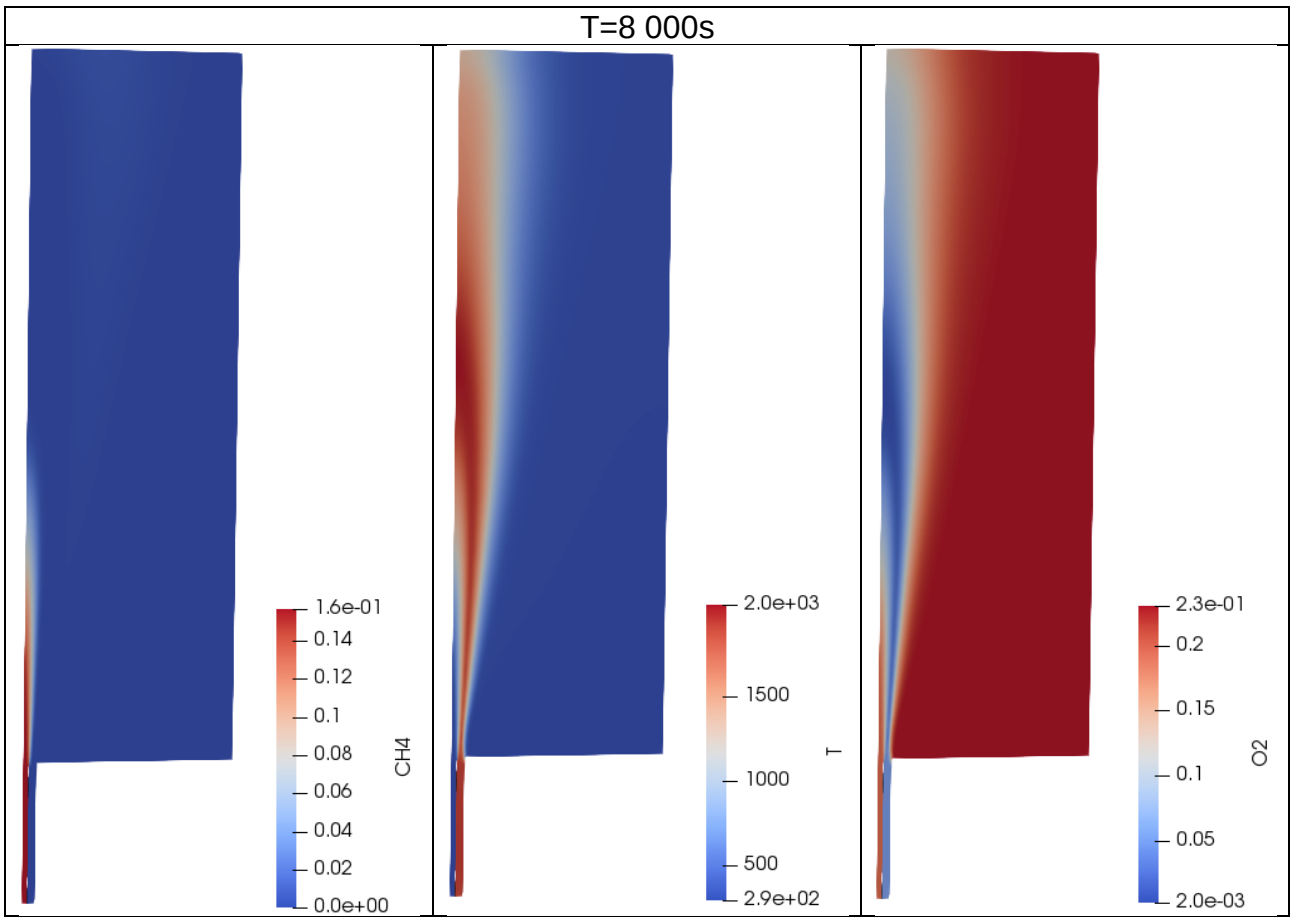
Figure 7 Mesh scope

Mesh refinement provide for more accurate solution e.g., scalars, velocity fields and improve quality of solution. From the other hand it can be treated as compromise between the huge computational cost and accuracy. In described case, the most interesting will be species mixing which influence directly on combustion process and on the temperature values.

First, calculations with settings written in files prepared by the use-case authors were carried on. In this way, achieved results were compared with the authors results noted in guide. After verifying that the files are compatible, calculation for first 1500s has been run without chemical reactions which means that there was no combustion. After that, flow field has been established and in combustion properties changes has been applied. The chemistry option has been switched from off to on. Results time step was set to 100s. Post processing were realized via paraview programe. There contours of CH_4, 0_2 fraction and temperature have been generated. All results from time step 0s, 1500s and 8000s have been placed in Table 3.

Table 3 Use-case results

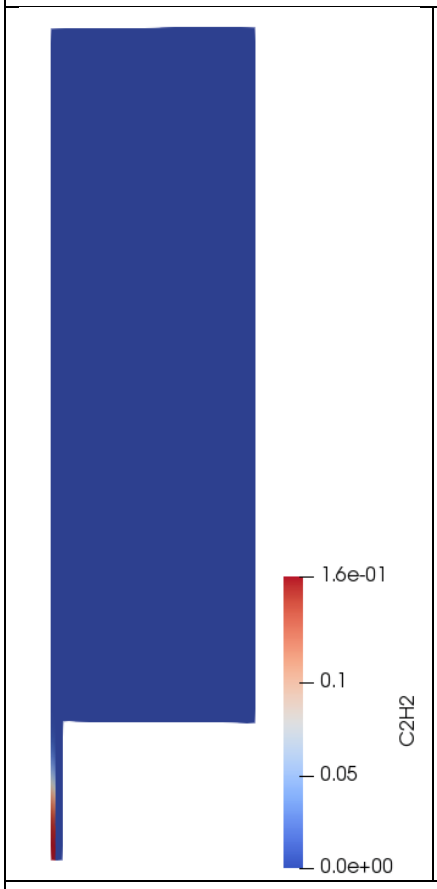
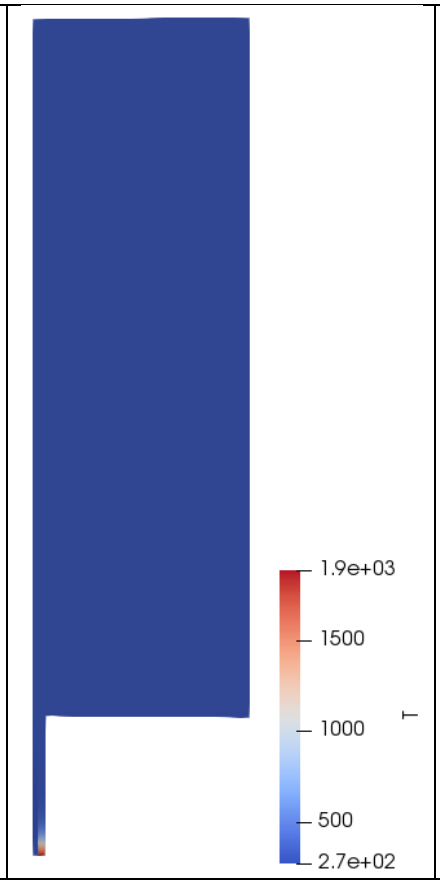
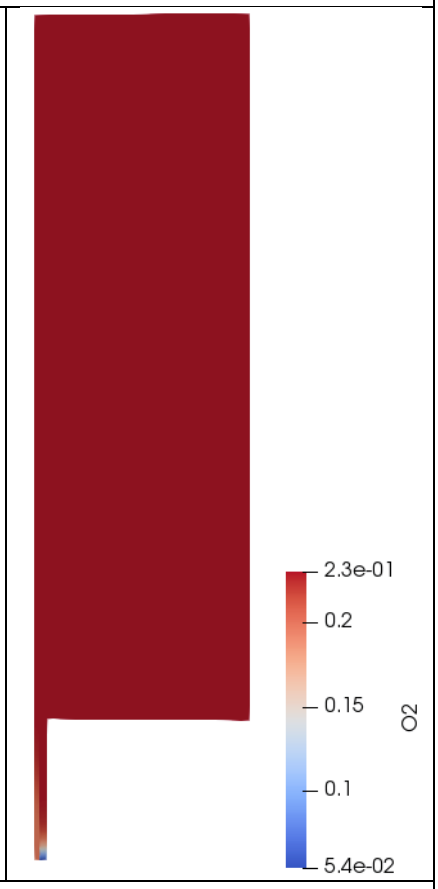
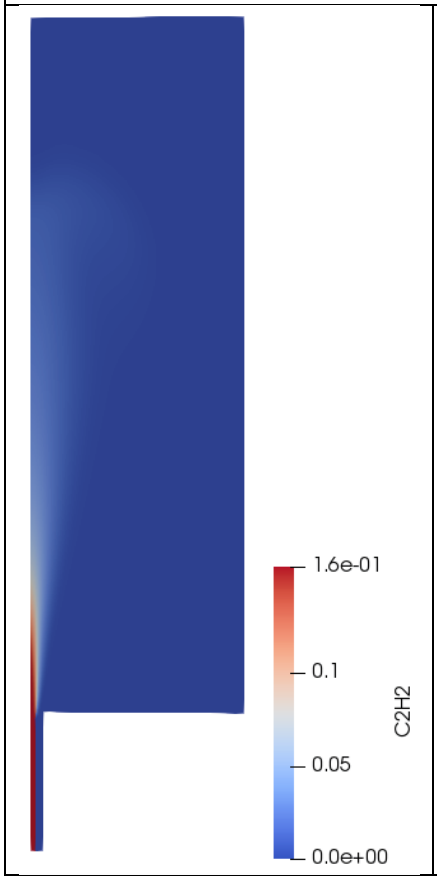
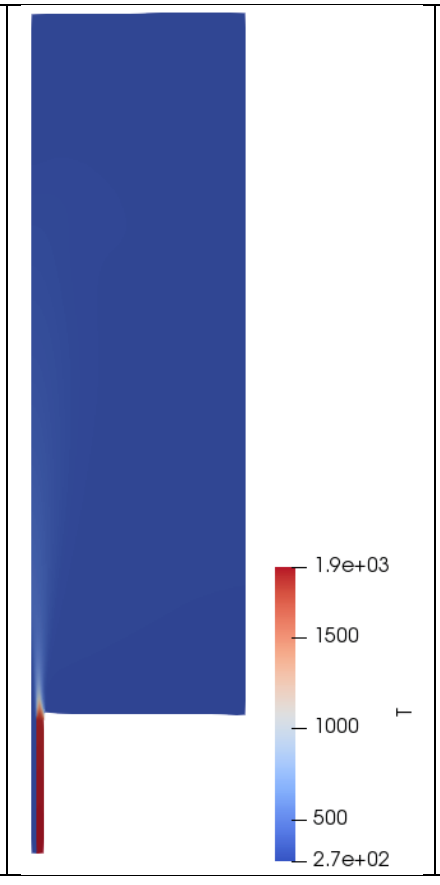
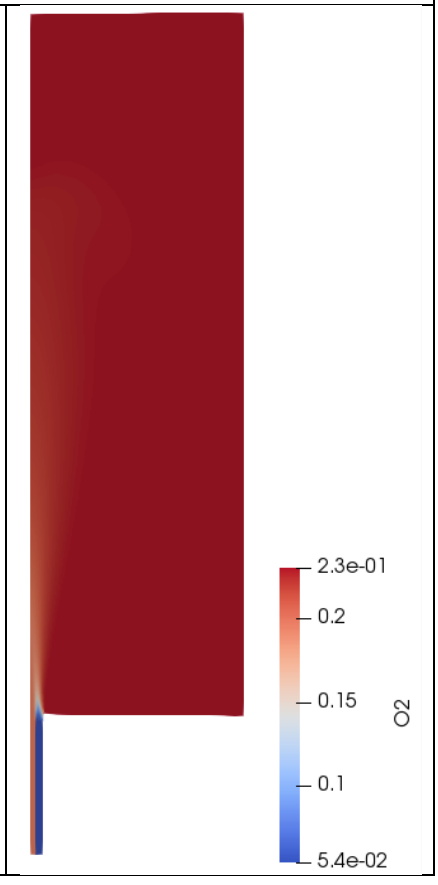
CH_4	T	O_2
T=0s		
		
T=1 500s		
		

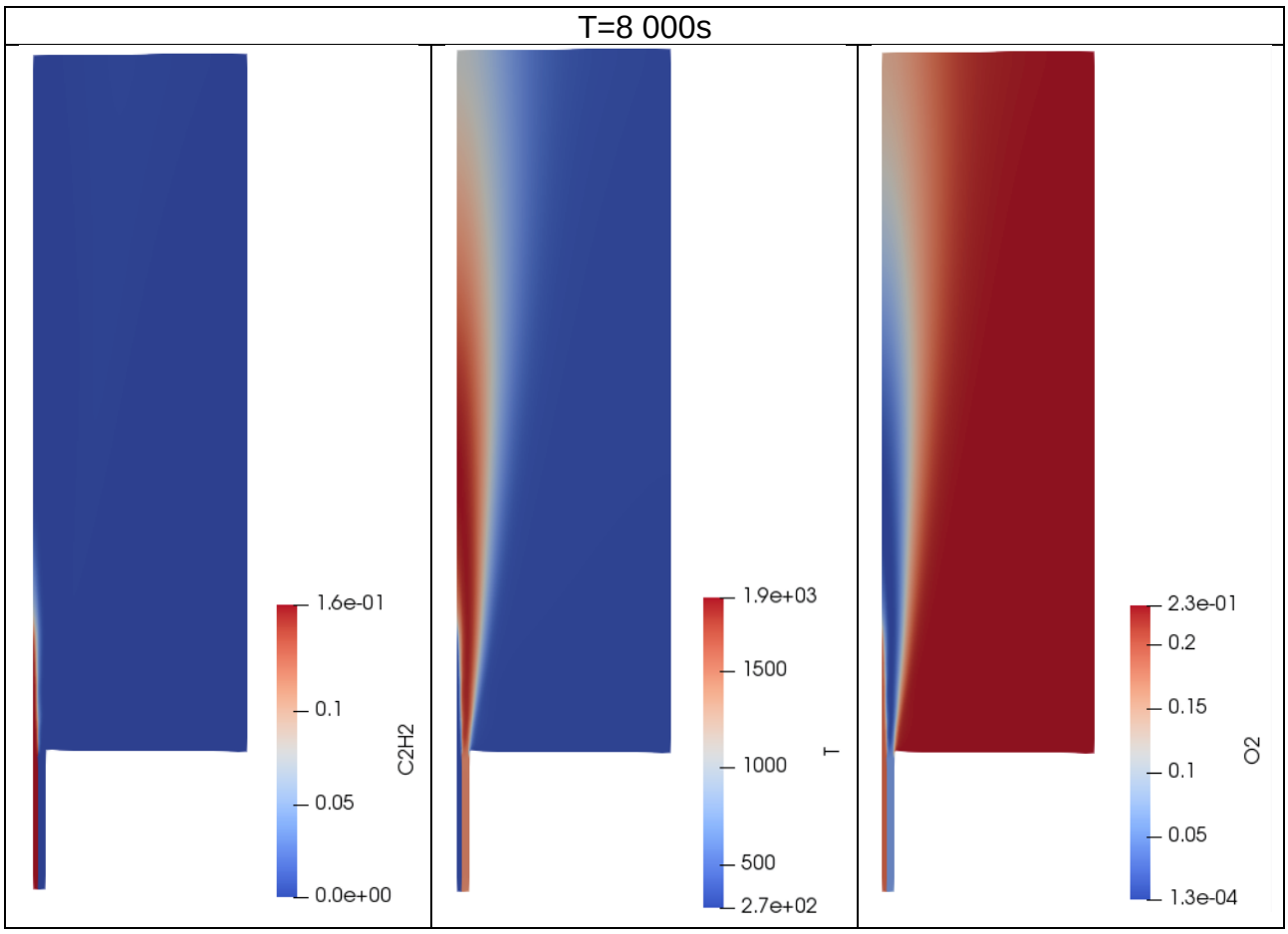


Modification

At the beginning C_2H_2 combustion possibilities were checked. The material at inlet has been changed. Inlet CH_4 mas flow has been changed for inlet C_2H_2 mass flow. Additionally whole 0 dictionaries including CH_4 has been changed for C_2H_2. C_2H_2 has been added as an important species inside the chemistryProporties dictionary. Rest of settings left unchanged. The same contour from the same time steps as for use-case results were collected in Table 4 C_2H_2 case results

Table 4 C_2H_2 case results

C_2H_2	T	O_2
T=0s		
		
T=1 500s		
		



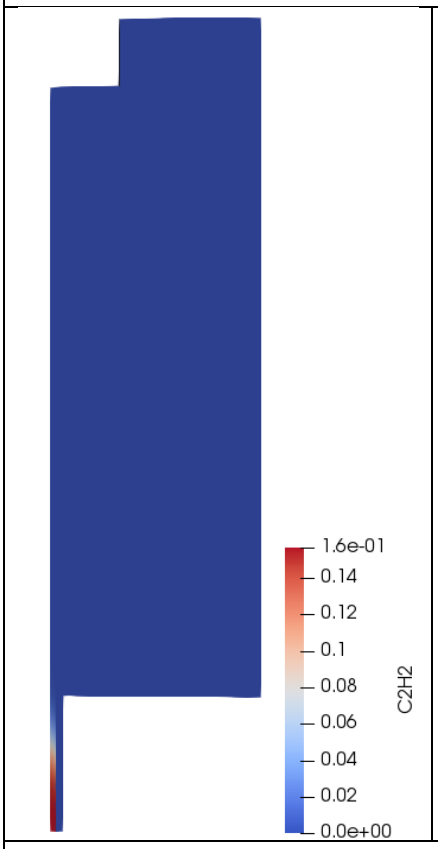
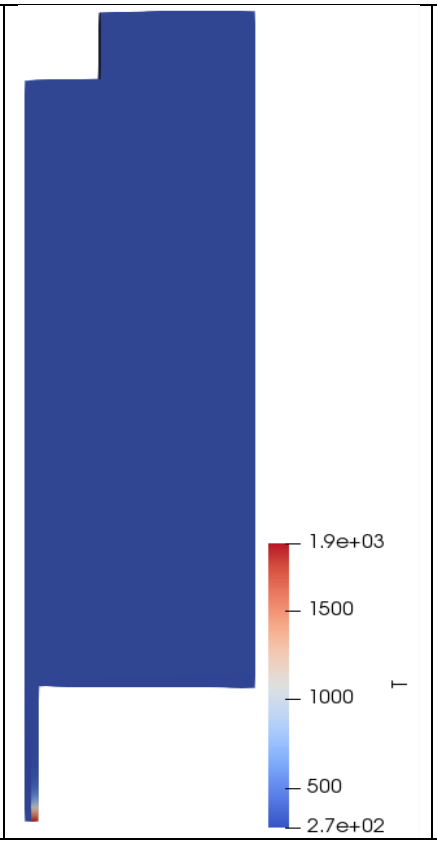
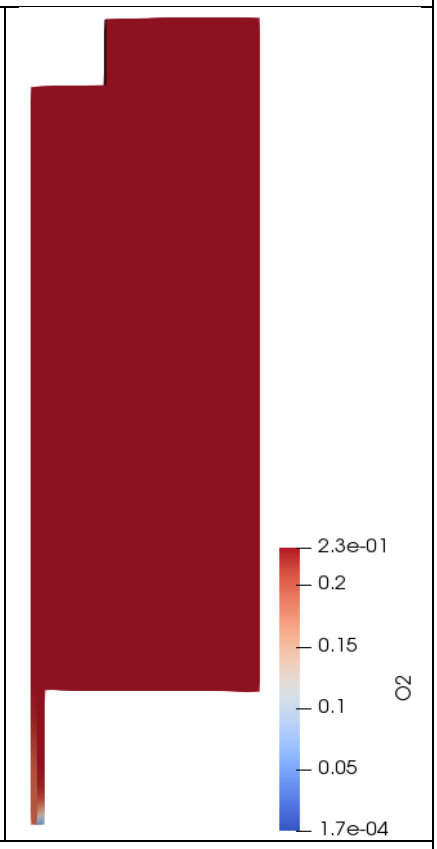
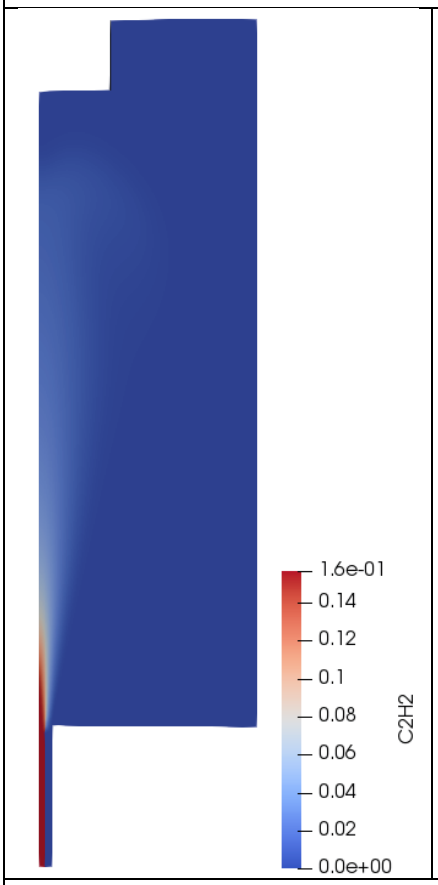
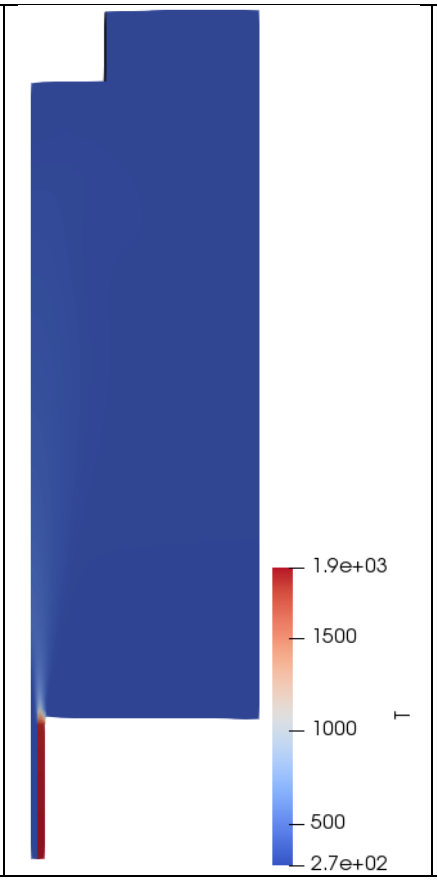
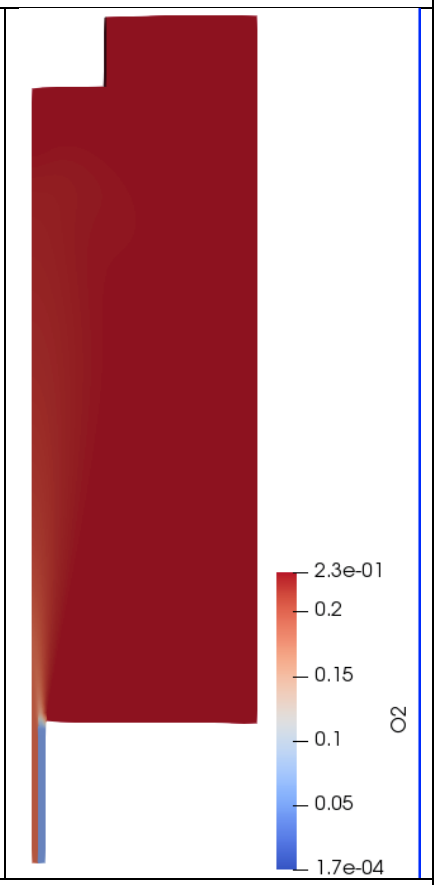
It was observed that with lowered solver time step size, calculations are stable and correctly solve case. Therefore, in next step, domain has been changed.

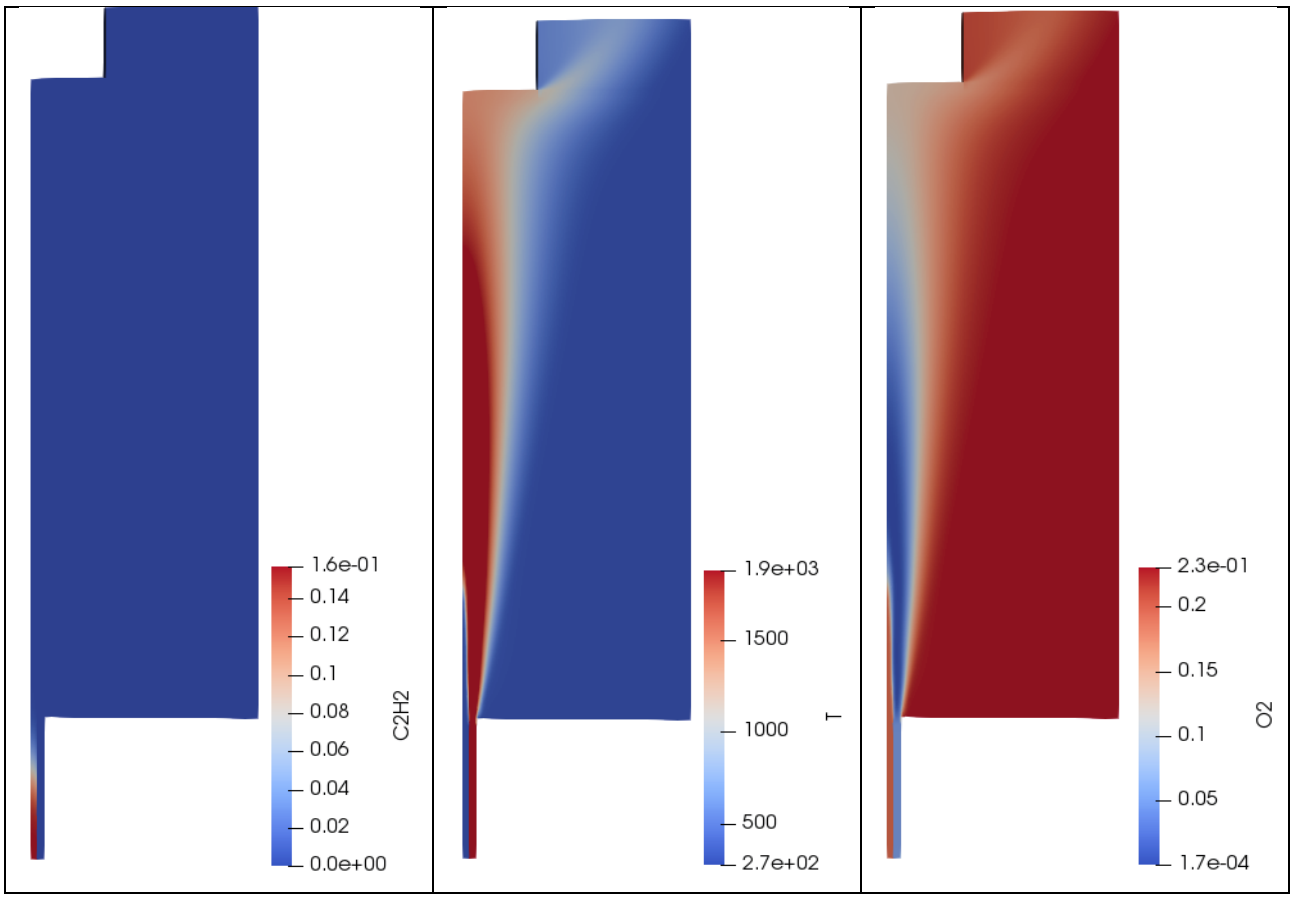
Based on [6] it was decided that the geometry will be change into a torch placed opposite solid body. The solid body is play role of a heat flux meter. Therefore, additional block to with φ100 x 50 had to be cut off from the domain Figure 8 with blockMesh dictionary usage.

Figure 8 Modified geometry

The same meshing method was used, mesh resolution left unchanged. Final results were presented in *Table 5.*

Table 5 Heat flux meter results

C_2H_2	T	O_2
T=0s		
		
T=1 500s		
		
T=8 000s		



Conclusion

Using open source, the OpenFOAM code it is possible to achieve results for transient solutions. Use-case prepared for the methane burner simulation has been modified to achieve case with acetylene torch. An interesting method for solution stabilizing has been suggested by the use-case authors. The proposition of switching chemistry properties is to allow the flow field to develop before starting the main simulation It can be noted that C_2H_2 fraction or CH_4 fraction contours for 1500s and 8000s time step clearly shows the difference between fuel concentration with and without combustion solver. It was noted that proposed reactingFoam returns reasonable results even for a combustion process with direct wall interaction. Lowered temperature for C_2H_2 cases is caused by lowered fuel mass which lowered air-fuel ration and disenabled to release the same amount of energy as in base case with CH_4.

Bibliography

[1] Standard Test Method for Oxyacetylene Ablation Testing of Thermal Insulation Materials, International Standard, 2015

[2] M.Rallini M.Natali L.Torre Nanomaterials in Rocket Propulsion Systems, Chapter 14 - An Introduction to Ablative Materials and High-Temperature Testing Protocols, Micro and Nano Technologies, ELSEVIER, 2019

[3] M. Aydin, Characterization of an Acetylene-Oxygen Flame for Material Studies on High-Temperature Materials, Master's thesis, Ruhr University Bochum, 2020

[4] Physical Parameters for Prediction of Transport Coefficients, Appendix B

[5] M. M. Borujeni, H. R. Norouzi, How to simulate combustion of a flame using OpenFOAM

[6] L. Fortner Numerical Investigation of an Oxyacetylene Torch Witch Regards to an Ablative Material, Master's thesis, University of Kentucky, 2022