13.06.2024
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Simulation of combustion in hybrid rocket motor

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1 Introduction

The main goal of this project was creating preliminary simulation of Nitrous dioxide (N_2O) and Acrylonitrile butadiene styrene (ABS) combustion. The simulation was conducted in Ansys Fluent. The main goal of this simulation was determining the areas of the highest temperature as it is critical information needed for proper design of combustion chamber.

2 Thermochemical data

In order to simulate combustion of ABS additional thermochamical data was added to fluent database. The additional data was added in the format of NASA-7 coefficient showed in equations 1 - 3 below:

$$\frac{C_p^o}{R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \tag{1}$$

$$\frac{H_T^o}{RT} = a_1 + \frac{a_2 T}{2} + \frac{a_3 T^2}{3} + \frac{a_4 T^3}{4} + \frac{a_5 T^4}{5} + \frac{a_6}{T} \tag{2}$$

$$\frac{S_T^o}{R} = a_1 \log T + a_2 T + \frac{a_3 T^2}{2} + \frac{a_4 T^3}{3} + \frac{a_5 T^4}{4} + a_7 \tag{3}$$

In order to simulate the combustion process it was assumed that due to the pyrolisysis process at 400K ABS break down into three of its main monomers in given mass fraction:

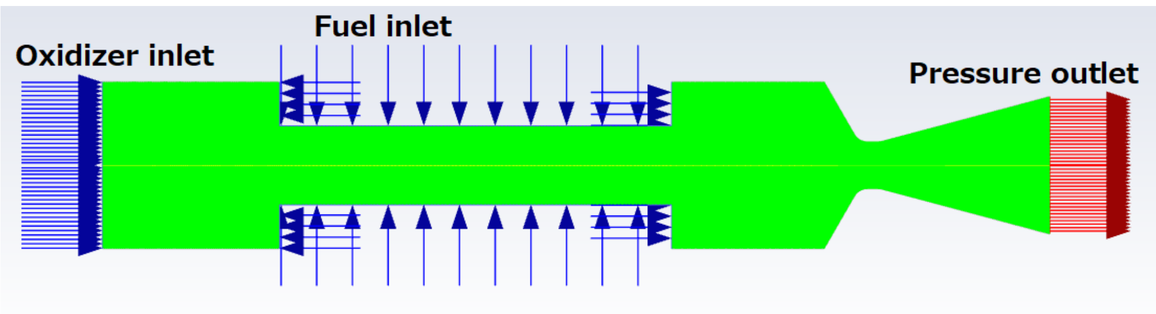
- Acrylonitrile (CH2CHCN) - 20%
- Butadiene (CH2=CH-CH=CH2) - 20%
- Styrene (C6H5CH=CH2) - 60%

The thermochemical data for each of those components was added to the fluent database. The values for the coefficient present in equations 1 - 3 were added from [1] and they are showned below:

```
C3H3N  CH2=CHCN              C    3H    3N    1      G    200.000    6000.000  1000.00      1
 6.52096861E+00 1.05028771E-02-3.73734374E-06 5.99498117E-10-3.57283503E-14    2
 1.92525453E+04-9.59580896E+00 3.04396646E+00 1.05333467E-02 1.96574996E-05    3
-3.42001077E-08 1.48155667E-11 2.06456740E+04 1.05816246E+01 2.21344883E+04    4
C8H8 styrene                 C    8H    8     0      G    200.000    6000.000  1000.00      1
 1.39192973E+01 2.94553961E-02-1.02697803E-05 1.31095793E-09-6.16742309E-14    2
 1.09344570E+04-4.97233295E+01 1.18176309E+00 3.34877555E-02 6.92369418E-05    3
-1.24490988E-07 5.49387246E-11 1.56039775E+04 2.26626016E+01 1.78362886E+04    4
C4H6                         C    4H    6     0      G    200.000    6000.000  1000.00      1
 7.62637466E+00 1.72523403E-02-6.09184911E-06 9.70800102E-10-5.76169721E-14    2
 9.55306395E+03-1.48325259E+01 4.10599669E+00 5.05575563E-03 5.83885454E-05    3
-8.05950198E-08 3.27447711E-11 1.15092468E+04 8.42978067E+00 1.33302095E+04    4
```

3 Domain

In order to create simulation 2D domain of hybrid rocket motor combustion chamber was created. The domain as well as boundary condition was presented on the figure 1

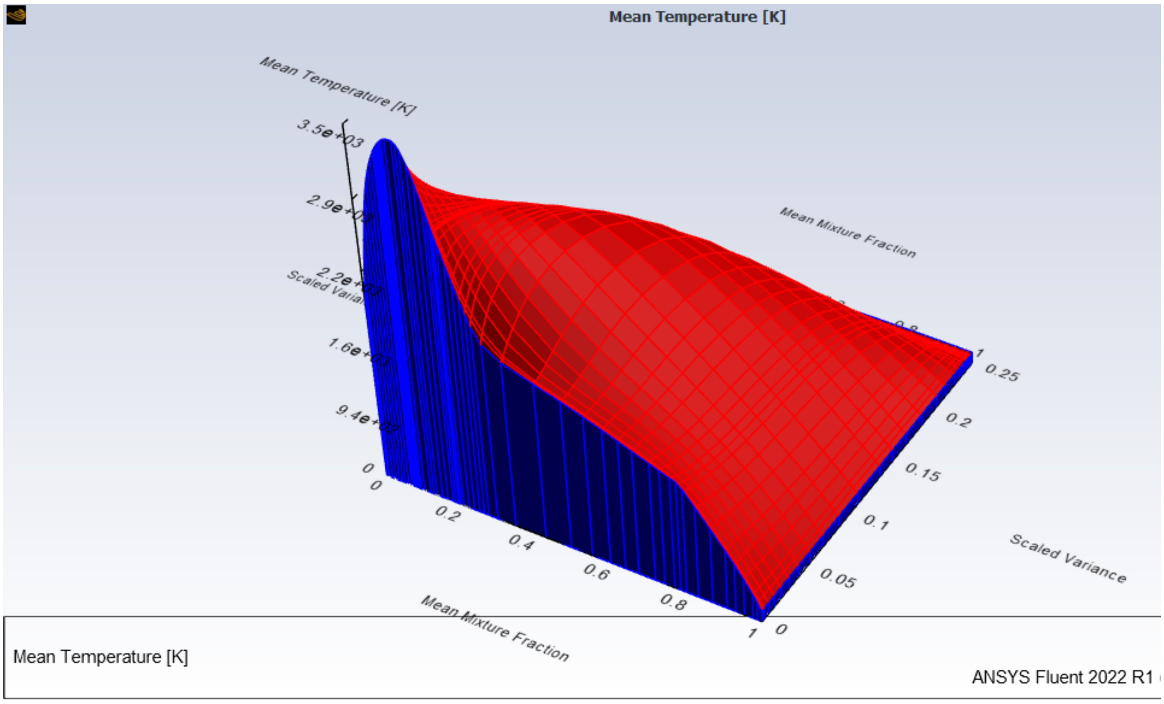


Rysunek 1: Domain and boundary conditions

4 Solution methods

4.1 Models

For the simulation the SST k-omega viscosity model was used. The combustion simulation was conducted using Non-premixed combustion model. the pdf-table for different combustion parameters was generated and can be seen on figure 2.



Rysunek 2: pdf-table for combustion parameters

As the non-premixed combustion model was used the calcualtions ere performed using pressure based solver.

4.2 Boundary conditions

For the boundary conditions given input data was choosen:

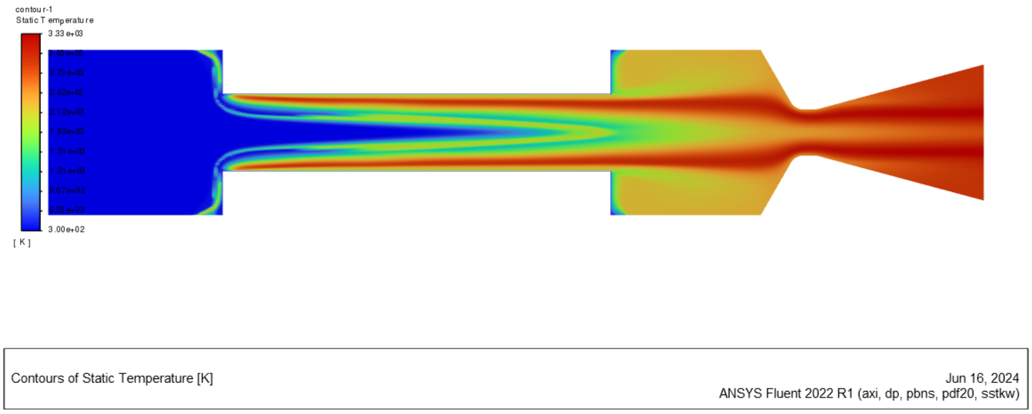
- Oxidizer inlet
  - mass flow rate: 0.2 [kg/s]
  - initial supersonic pressure: 30 [bar]
  - turbulent intensity: 5%
  - turbulent length scale: 0.017 [m]
  - Temperature: 300 [K]
- Fuel inlet
  - mass flow rate: 0.03 [kg/s]
  - turbulent intensity: 10%
  - turbulent viscosity ratio: 10%
  - Temperature: 400 [K]
- Pressure outlet
  - Gauge pressure: 0 [bar]

4.3 Methods

For the simulation coupled solver was used, the simulation were performed by using firstly the first order solution methods and after achieving reasonable results the simulations using second order solution methods were condusted.

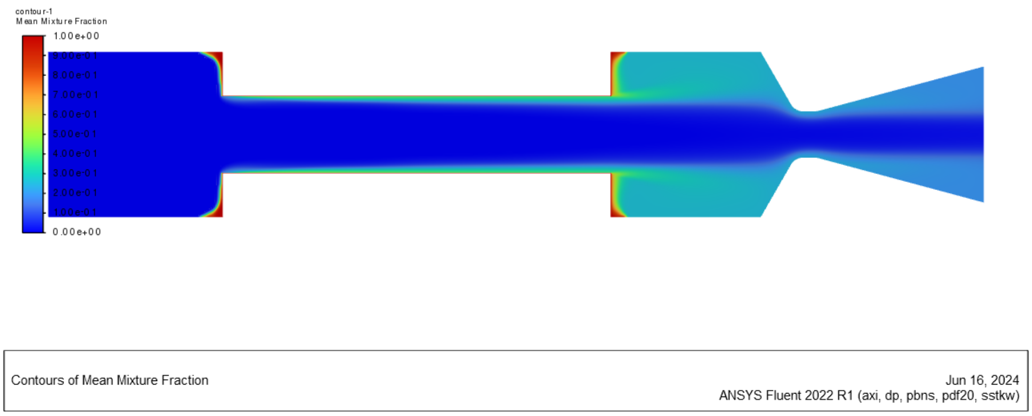
5 Results

5.1 Temperature profiles



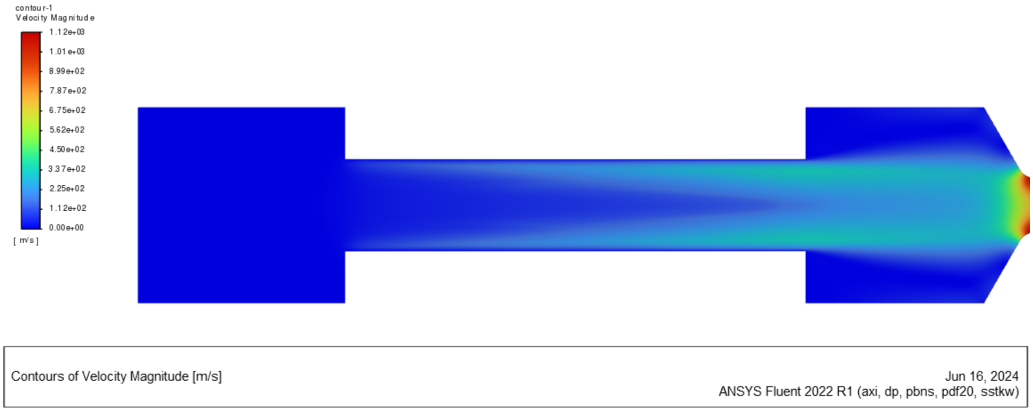
Rysunek 3: Mean temperatures inside combustion chamber

5.2 Mean mixture frctions



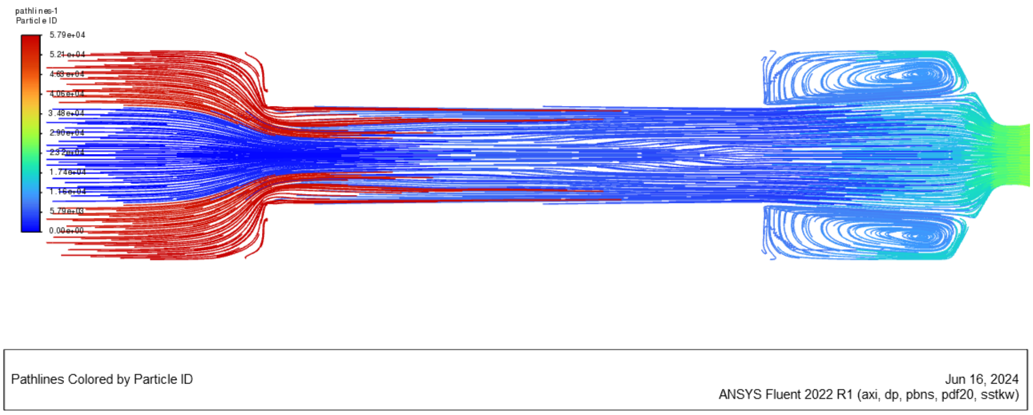
Rysunek 4: Mean mixture fractions inside combustion chamber

5.3 Velocity



Rysunek 5: Mean velocity inside combustion chamber

5.4 pathlines



Rysunek 6: Pthlines of the flow inside combustion chamber

6 Conclusions

We can see the formation of the flame inside the grain canal form the mean temperature contur. The highest noted temperature inside the combustion chamber can be located in the thie grain canal flame and is around 3300 [K].in the post combustion chamber we can see the recirculation region. The highest fraction of the fuel can be found o the grain face as well as near walls where smaller recyrculations regions shield fuel vapors from being burn ith the oxidizer. In order to get better results the domain outside the nozzle could be simulated as current flow through the nozzle is not accurately represented due to usage of pressure based solver.

Bibliografia

- [1] Alexander Burcat and Branko Ruscic "Third Millennium Ideal Gas and Condensed Phase Thermochemical Database for Combustion with updates from Active Thermochemical Tables"TAE 960; ANL-50/20 Technion-IIT, Aerospace Engineering, and Argonne National Laboratory, Chemistry Division, 2005.
- [2] Comparing Hydroxyl Terminated Polybutadiene and Acrylonitrile Butadiene Styrene as Hybrid Rocket Fuels Stephen A. Whitmore, Zachary W. Peterson,† and Shannon D. Eilers† Utah State University, Logan, Utah 84322
- [3] Ansys Fluent User guide