Oxy-combustion simulation of ethylene

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Abstract. The paper presents the simulation of the combustion of ethylene intended to be used in hybrid rocket propulsion. The simulation, was performed in ANSYS numerical codes, considering the following assumptions: fuel temperature 700 K and 800 K, pressure in the combustion chamber 1 to 3 bar; overall excess air from 1.5 to 5, in order to determine the case with lowest pollutant species. The simulation displayed the combustion temperature field, the flame OH concentration field, the exhaust gases composition fields, the gases velocity field, NO, CO, CO₂ concentration fields and the gases pressure field. The simulation showed the influence of fuel temperature upon the combustion spatial features.

1. Introduction
Fuels for hybrid rocket engines have some advantages in comparison to pure solid or liquid propellants, including increased safety regarding storage feeding system, propellant versatility, much simple design solution, low temperature sensitivity, and low relative cost. Although there are some disadvantages regarding low volumetric loading, potential fuel residuals, mixture ratio shift during motor firing, and mixing and combustion inefficiencies [1]. The most commonly cited drawback of their performance is actually low solid fuel regression rates. Research efforts devoted to overcoming these drawbacks have led to numerous fuel regression rate enhancement strategies including utilization of non-traditional fuels and oxidizers; manipulation of oxidizer flow to yield unique flows, such as swirl or vortex flows; inclusion of energetic additives such as metals, metal hydrides, and solid oxidizers; and augmentation of combustion port geometry to yield increased burn surface area. Compared to a liquid fuel system, the hybrid fuel system presents the advantage of a reduced explosion hazard and complexity due to the absence of regenerative cooling systems used for the combustion chamber and nozzle [2].

2. Combustion basic chemistry of ethylene
One hybrid rocket engines fuel used is polyethylene. Main combustible product obtained after ethylene pyrolysis process in hybrid rockets is ethylene. Thus, in this paper is presented a simplified simulation model of ethylene combustion process using pure O₂ as oxidizer. Few researches had been carried out in order to improve the knowledge of ethylene oxidation. In the paper [3], there were detailed some measurements of the laminar flame velocity of ethylene-air mixture. For some intermediate temperatures there were some studies using jet stirred reactors to derive analytical data [4, 5]. In the works [7-10] there were included studies regarding ethylene flame chemical composition at low and atmospheric pressure, using mass spectrometer.
At intermediate temperatures most reactions between C\textsubscript{2}H\textsubscript{4} and chemical radical species like O and OH including reactions (1), (2), and (3), appear to involve the formation of an activated complex followed by a rearrangement and subsequent fragmentation [9].

The rates and product distributions for reactions between ethylene and O, OH and H radicals have been the subject of considerable study. At high temperatures abstraction reactions can be expected to be important, including reactions (4) and (5).

\[
\begin{align*}
C_2H_4 + O &\rightarrow CH_3 + HCO \\
C_2H_4 + O &\rightarrow CH_2O + CH_2 \\
C_2H_4 + OH &\rightarrow CH_3 + CH_2O \\
C_2H_4 + OH &\rightarrow C_2H_3 + H_2O \\
C_2H_4 + OH &\rightarrow C_2H_3 + H_2O
\end{align*}
\]

3. Combustion chamber design and ANSYS model

In order to analyse the oxidation process of ethylene was designed a simplified model of a combustion chamber with one oxidizer inlet located in the front, four fuel inlet ports located on the circumference of the combustion chamber and one outlet port for flue gases. Combustion chamber model have a length of 200 mm and diameter 52 mm.

For these simulations was used ANSYS software, in order to create the mesh and to define all the necessary input computational parameters of combustion process. To obtain a simplified model and shorter computational periods there were removed all components of the combustion chamber like walls, fixtures, spark plug, etc. The meshed model was developed on the inner volume of combustion chamber, and defined the inlet and outlet flow areas. The mesh has 335000 elements and 64682 nodes with finite element sizes of 1 mm. The mesh has a refinement in the oxidizer inlet area and fuel inlet area. They were assessed numerical simulations of reactive turbulent flow through the combustion chamber of ethylene burning, using pure O\textsubscript{2} as oxidizer. Using ANSYS CFX-RIF module they were defined the reactions for ethylene combustion using O\textsubscript{2}. The carried out simulations used excess oxygen ratios of 1.5 and 3, fuel temperature of 700 K and 800 K. The presumed combustion pressures were set for 1 bar, 2 bar and 3 bar. Oxidizer inlet temperature was set at 300 K.

The adopted oxidizer inlet flow area has a round shape and 12.99 cm\textsuperscript{2}. The fuel, pure C\textsubscript{2}H\textsubscript{4}, enters the combustion volume using four circular inlets with a total area of 1.319 cm\textsuperscript{2}. The fuel mass flow rate is set to 1.169 x 10\textsuperscript{-4} kg/s.

The imposed selected chemical reactions and used in the combustion simulations are:

\[
\begin{align*}
C_2H_4 + 3O_2 &\rightarrow 2CO_2 + 2H_2O \\
2CO_2 &\rightarrow 2CO + O_2 \\
CO_2 &\rightarrow CO + O \\
2H_2O &\rightarrow 2OH + H_2 \\
H_2O &\rightarrow OH + H \\
CO_2 + H_2 &\rightarrow CO + H_2O
\end{align*}
\]

All carried out simulations meet the convergence criteria after minimum 2500 computational steps.

4. Simulation results.

Below figures, 1 to 12, depict the temperature fields, the velocity fields, and spatial mass fractions of chemical species C\textsubscript{2}H\textsubscript{4}, CO, CO\textsubscript{2} and NO, for each imposed values of pressure, excess oxygen ratio, and fuel temperature for two demonstrative cases.
4.1. Fuel temperature 800 K, excess oxygen ratio 1.5, pressure 3 bar

Analysing the figure 2, it is visible that the flow reactive process has the following aspects:

- a laminar profile after the fuel injector ports toward flue gases outlet, and
- around the oxidizer inlet appears a backflow causing an intense recirculation of hot combustion products inside combustion chamber.

These particular aspects have strongly affected the other parameters fields inside combustion chamber.
4.2. Fuel temperature 800 K, excess oxygen ratio 3, pressure 3 bar

The velocity field, figure 8, is characterised by a laminar flow, and therefore the temperature field has highest temperatures in the centre of combustion chamber. In order to obtain a more homogeneous combustion process it is necessary to use inlet flow geometries causing artificial turbulence.

The next below figures include the average values of NO, CO, CO₂ mass fractions, measured on the outlet section of combustion chamber. These averaged values were recorded in 25 points on this flow section. Figure 13 shows the presence of NO mass fraction, with highest value in the case of simulation with 800 K fuel temperature, excess oxygen ratio of 1.5 and pressure of 1 bar. The lowest values of NO mass fraction were obtained in the case of 700 K, excess oxygen ratio of 3, and pressure of 3 bar.
Figure 13. NO mass fraction for analyzed cases.

The Figure 14 includes the average mass fraction of CO in same points. Minimum value of CO mass fraction is obtained in the case of 700 K, excess oxygen ratio of 1.5, pressure of 1 bar, and maximum value is obtained in the case of 800 K, excess oxygen ratio of 1.5, pressure of 3 bar.

Figure 14. CO mass fraction for analyzed cases.

Figure 15 shows the average CO$_2$ mass fraction, with highest value in the case of simulation with 700 K fuel temperature, excess oxygen ratio of 3 and pressure of 3 bar. Lowest value for this mass fraction is obtained in the case of 700 K, excess oxygen ratio factor 1.5, and pressure 1 bar.

Figure 15. CO$_2$ mass fraction for analyzed cases.
5. Conclusions
After conducted simulations some conclusions are revealed. In order to obtain a more homogeneous combustion process it is necessary to use inlet flow geometries causing artificial turbulence. Minimum value of CO mass fraction is obtained in the case of 700 K, excess oxygen ratio of 1.5, pressure of 1 bar, and maximum value is obtained in the case of 800 K, excess oxygen ratio of 1.5, pressure of 3 bar. Minimum NO mass fraction concentrations are obtained in the case of 700 K, excess oxygen ratio of 3, and pressure of 3 bar, while highest value is obtained in the case of simulation with 800 K fuel temperature, excess oxygen ratio of 1.5 and pressure of 1 bar. For CO\(_2\) mass fraction concentration, the highest value is obtained in the case of simulation with 700 K fuel temperature, of 3 and pressure of 3 bar while the lowest value is obtained in the case of 700 K, excess oxygen ratio 1.5, and pressure 1 bar.

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