CFD Analysis of Melt-Layer Characteristics during Combustion of Cryogenic Methane as Hybrid Rocket Fuel

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ABSTRACT

Cryogenic hybrid rocket fuels are a class of fuels that forms a melt layer of low viscosity and low surface tension on the solid surface during combustion. Under the influence of oxidizer flow conditions some of the fuel droplets from the melt layer entrained in the oxidizer flow, thus increasing the regression rate of the fuel. In order to get the in-depth details, numerical code has been developed to simulate the flow in hybrid rocket engine with cryogenic methane with real gas equation of state.

Introduction Hybrid Rockets:

Hybrid rocket engines emerged from the combination of the solid and liquid rocket engines. The primary characteristic of the hybrid rocket engine is that the fuel and oxidizer are stored in the different storage tanks and in different phases. In the conventional hybrid system, the oxidizer (liquid) is kept in the different tank. Whereas the fuel (solid) is kept, inside of the chamber which also acts as a combustion chamber. Due to the flow of liquid oxidizer over the inner surface of the fuel grain, boundary layer forms and the combustion flame which is also called diffusion flame forms inside this boundary layer. The position of the diffusion flame depends on the mass ratio of oxidizer and fuel available at the specific position in the domain. Heat from the flame convect towards the fuel. First, it is used for the pyrolysis process inside the fuel grain and then for the evaporation of the fuel from its surface. The oxidizer is transported from the mean stream-flow.



Fig.1. Hybrid rocket configuration

Advantages:

• Eco-friendly, combustion products are less polluting.

- Since, oxidizer and fuel are stored in different storage and phase, hybrid rockets are nearly non-explosive.
- Only oxidizer is in liquid phase which decreases the requirement of complex pumps and pipes. So, low cost of manufacturing.
- Hybrid engines are throttleable and can be extinguished in the scenario of emergency.
- Grain robustness: Fuel grain cracks are not catastrophic as the combustion only occurs where fuel encounters the oxidizer flow.

Disadvantages/Limitations:

- Low fuel regression rate, due to the nature of diffusion flame.
- Low bulk density, to increase the regression rate more fuel surface is required, which results in the use of multi-port fuel grain. This can lead to the low volumetric loading of the fuel.
- With time port area increases and results into the O/F shift.
- Combustion efficiency because of lower degree of mixing

Combustion mechanism:

Gas flow in the hybrid rocket engine is like the flow in the circular pipe, but here flow is confined in the port of the fuel. For the simplicity, it can be visualized as the flat plate flow where oxidizer flows over the fuel surface. The flow forms a reacting boundary layer over the fuel surface. This boundary layer has a strong temperature, velocity, and chemical species gradients and contains a diffusion flame inside of it.



Fig.2. Combustion process schematic of hybrid rocket engine [1]

Heat from the flame convects and radiates towards the fuel surface. Transportation of the oxidizer towards the flame is from the mainstream flow. But fuel transportation takes various steps which depends on the type of fuel. Usually, sublimation and pyrolysis take place in conventional fuels. In the pyrolysis solid to gas phase change takes place along with the chemical change, such as polymer chain breaking, cyclization, and re-organization that takes place inside of the fuel grain near to surface. However, there are other fuels like solid cryogens (cryogenic methane) which melt or sublimate without any chemical change. Whereas paraffinbased fuels form a melt layer over the solid fuel surface and combustion takes place with an interesting phenomenon called entrainment where fuel sprayed in the form of droplets along with the gasification towards the diffusion flame.

Blocking effect:

During hybrid rocket combustion one interesting phenomenon takes place called blocking effect. It is the tendency of the vaporizing fuel mass flux to block the incoming heat flux coming from the flame. This means that even trying increasing regression rate by increasing heat flux to the fuel surface will end up increasing the blocking effect, which in turn tend to decrease the regression rate. Simplified fuel regression rate is given by:

$$\rho_f r = 0.036 \text{GB}^{0.23} \text{Re}_{\text{x}}^{-0.2}$$

Here, G is the total mass flux, and B is the blocking number which is defines as follows [2]:

$$B = \frac{h_{fl} - h_w}{\Delta H_{v.eff}}$$

It describes the enthalpy driving force between the flame and the fuel surface which causes the fuel regression. Increasing the enthalpy difference can increase the fuel regression rate which will facilitate the blockage of convective heat transfer. This is a tight coupling between the solid-fuel regression rate and the aerodynamics of reacting boundary layer flow [2].

Need of cryogenic fuels/liquefying fuels:

Blocking effect is an aerodynamic behavior and is caused only by the gaseous flow. In the case of cryogenics, fuel travels in a different manner. In this case melt layer forms on the surface of these fuels which becomes unstable under the influence of main stream flow conditions. Instability gives rise to the formation of the roll waves on melt layer which injects fuel droplets toward the diffusion flame. Spraying of fuel droplets is called as entrainment.

Droplets doesn't participate in blocking effect. These fuels have been already tested and successfully shown the 5-6 times increase of regression rate as compared to conventional fuels [3].



Fig.3. Entrainment mechanism ©Stanford.edu

Regression rate in liquefying fuels can be summarized as:

Regression Rate=Entrainment+ Vaporization

$$m_{ent} \propto \frac{P_d^{\alpha} h^{\beta}}{\sigma^{\pi} \mu_l^{\gamma}}$$

Here, *P* is Pressure, *h* is melt-layer thickness, σ is surface tension, μ is dynamic viscosity of the liquid layer, and exponents α , β , γ , and π are the constants specific for a fuel.

Fuel Selection:

The primary focus for the selection of fuel was on the fuels with strong entrainment capability under the practical hybrid engine operating conditions. Initially, a whole range of n-alkanes hydrocarbons was available, which can be divided into 3 major categories. Cryogenics, Waxes, and High-Density Polymers (HDPE).

The melt layer in the HDPE is too dense with high viscosity which makes entrainment impossible. Hydrocarbons up to PE waxes could have been selected but the combustion computation with longer chain molecules becomes very complex because of the thermal cracking of the polymer chains. Therefore, I restricted my choice to simpler n-alkanes and selected CH_4 as the fuel, the most basic hydrocarbon.



Fig.4. Entrainment in n-alkane hydrocarbons [4]

In liquefying fuels entrainment onset parameter can predict the entrainment possibilities [5].

$$a_{onset} = 1.05 \times 10^{-2} \left[\frac{\rho_g^{1.3}}{\rho_l^{0.3}} \right] \frac{1}{\left(C_{fref} C_{B1} \right)^{0.8}} \left[\frac{1}{\mu_g} \right] \sigma \mu_l^{0.6}$$

Here, ρ is density of melt layer and the mainstream gas, C_{fref} is coefficient of friction, μ is the viscosity and σ is the surface tension.

 a_{onset} should be less than 0.4 for any fuel to show entrainment.

 α_{onset} for methane and oxygen system was calculated and it came out be ≈ 0.14

Real Gas Equation of State:

For the treatment of real gas effects in the computational domain, Peng-Robinson Equation of State (PR-EOS) was selected and tested with various calculation considering Methane fluid. Departure functions are one of the most important variables which are specific to any equation of state. Departure functions quantify the departure of any property in the real world from the ideal gas state.

Results:

Peng-Robinson EOS Analysis:

PR-EOS has been used to analyzed different thermodynamic properties of Methane at 5 MPa and the temperature range capturing subcritical as well supercritical state.



Fig.5. Density of CH₄ at 5 MPa.



Fig.6. Specific heat of CH₄ at 5 MPa

Simulations:

Simulations were done with developed laminar CFD solver on the 2-D flat plate which is capable of mimicking the flow over the fuel surface in hybrid rocket engine.

Uniform mesh has been used to discretize the computational domain. AUSM scheme has been used for convective fluxes.

Computational domain:



Fig.7. Computational domain

Several cases have been considered for the simulations which are as follows:

| | Case 1 | Case 2 |
|-------------|-----------------|-----------------|
| Fluid(s) | CH ₄ | CH ₄ |
| Boundary | | |
| Conditions: | | |
| Wall | No-slip | No-slip |

| Inlet | Constant | Constant |
|-----------|--------------|--------------|
| | mass flow at | mass flow at |
| | 0.1 Mach | 0.1 Mach |
| Outlet | Constant | Constant |
| | pressure | pressure |
| | (0.1 MPa) | (0.1MPa) |
| Far-Field | Symmetry | Symmetry |
| EOS | IEOS | PR-EOS |
| State | Subcritical | Subcritical |
| | | |

Table.1. Simulation conditions

Here, EOS (Equation of state), IEOS: Ideal EOS, PR-EOS: Peng-Robinson EOS.

Case 1.



Fig.7. Axial velocity at 0.6 m



Fig.8. Axial velocity contour in the domain





Fig.9. Axial velocity at 0.12 m

Conclusion:

- CFD solver has been developed with AUSM scheme capable of capturing real gas effects with Peng-Robinson equation of state.
- Developed CFD solver performed well with IEOS as well as with PR-EOS.
- PR-EOS gave satisfactory results in the simulations.

Future Works:

- On the basis of PR-EOS performance, it could be selected for the more comprehensive analysis of liquefying fuels combustion in hybrid rocket engine.
- Melt-layer characteristic and the behavior of fuel droplets could be investigated in an elaborated way.

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