CFD Simulation of Hybrid Rocket Motors for Interplanetary CubeSats


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Abstract
This paper presents the results of a Computational Fluid Dynamics analysis on a gaseous oxygen/polymethyl methacrylate hybrid rocket motor. This analysis supports the current research at NASA’s Jet Propulsion Laboratory to develop a high performance, compact propulsion system for an Interplanetary CubeSat/SmallSat. The analysis presented here was conducted to give insight into the performance versus mass trade for the final design. Experimental data have been post-processed through an in-house tool and have been used to validate Computational Fluid Dynamics analysis outputs. The benefit of adding a post-combustion chamber has been investigated as a way to increase performance.

Nomenclature

\( A \) area
\( \tilde{A} \) Standard Eddy Break-Up model parameter
\( \tilde{B} \) Standard Eddy Break-Up model parameter

CEA Chemical Equilibrium with Applications
CFD computational fluid dynamics
CFL Courant Friedrichs Lewy

\( D \) diameter m

EBU Eddy Break-Up model

\( \eta \) combustion efficiency

\( F \) fuel

\( F_{\text{thrust}} \) N

GOX gaseous oxygen

\( h_{\text{e}} \) effective heat of gasification kJ/kgK

\( L \) fuel length m

\( M \) molecular weight g/mol

\( m_{\text{o}} \) oxidizer mass flow rate kg/s

MMA methyl methacrylate

O oxidizer

\( \text{OF} \) oxidizer to fuel ratio

P product

\( p_{\text{c}} \) mean chamber pressure Pa

pcc post-combustion chamber

PMMA polymethyl methacrylate

\( \dot{Q} \) heat flux W/m²

\( t_b \) burn time s

\( \dot{r} \) regression rate mm/s

T temperature K

\( u \) velocity m/s

\( \bar{Y} \) mass fraction

\( z \) longitudinal location m

\( \epsilon \) dissipation rate \( m^2/s^3 \)

\( k \) turbulent kinetic energy \( m^2/s^2 \)

\( \nu \) stoichiometric coefficients of reacting species

\( \tau_R \) time scale s

\( \rho \) density kg/m³

\( \Delta p \) pressure drop Pa

\( \Delta h \) enthalpy difference between the flame and the wall kJ/kgK

Subscript

\( c \) combustion chamber

\( \text{cond} \) conductive

\( \text{conv} \) convective

\( e \) external

\( f \) final

\( i \) initial

\( \text{inj} \) injection

\( j \) generic index

\( \text{lit} \) literature

\( \text{pyr} \) pyrolysis

\( \text{rad} \) radiative

\( \text{stoic} \) stoichiometric

\( t \) throat

\( w \) fuel wall surface

\( 0 \) ambient

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1. Introduction

Hybrid rocket motors represent a promising alternative to conventional propulsion systems due to their increased safety and decreased complexity and cost.\textsuperscript{3–5} A hybrid propulsion test facility has been built at NASA Jet Propulsion Laboratory.\textsuperscript{6, 17} The current focus of this research is developing a propulsion system for an Interplanetary CubeSat/SmallSat.\textsuperscript{12} More than 50 tests have been performed with different propellant combinations and motor configurations. PolyMethyl MethAcrylate (PMMA) and Gaseous Oxidizer (GOX) were determined to be the best propellant combination for the interplanetary cubesat application.

The focus of the presented work is to investigate the behavior of the internal fluxes to inform the final design of the hybrid motor. Numerical simulations of hybrid rocket motor internal fluid dynamics have been carried out on STAR-CCM+, a Computational Aided Engineering solution for solving multidisciplinary problems in both fluid and solid continuum mechanics. The STAR-CCM+ computational fluid dynamics outputs have been validated through experimental data. A step-by-step method has been adopted, to validate incremental pieces of motor behavior. First, the combustion process between the two selected propellants PMMA/GOX has been analyzed in depth to define a satisfactory combustion model. Once the combustion model was validated, it was applied to analyze performance of the hybrid rocket motor. Two hybrid rocket motor configurations have been analyzed to understand the effect of design variations on performance: a nominal configuration and a configuration with post-combustion chamber. Flow altering devices and tailored post-combustion chamber designs can be used in hybrid rocket motors to enable more complete burning of the combustion products before they are expelled through the nozzle. However, they can cause quite severe erosion of the aft end of the combustion chamber and the benefit can be outweighed by the increased mass of the insulation required.\textsuperscript{1} A parallel thermal study has been also performed at Jet Propulsion Laboratory to evaluate the temperature in the motor, especially in the post-combustion chamber.\textsuperscript{7}

1.1 Hybrid Rocket Motor Design

Capabilities and design of the JPL hybrid propulsion test facility are discussed in Ref. 6, 17. Constraints of the system are fuel grain outer diameter (0.051 m), maximum expected operating chamber pressure (2.4 MPa), maximum oxidizer upstream pressure (6.89 MPa). A differential pressure transducer is used to control and measure the oxidizer mass flow rate and it is located upstream of the injector. Two pressure transducers are located at the fore end cap of the motor, see Figure 1.

![Pressure Transducers](image)

Figure 1: Hybrid rocket motor, hybrid rocket facility 2016.

As mentioned previously, two motor configurations have been tested; these are shown in Figure 2. The nominal design has a convergent-divergent nozzle right after the fuel grain. This configuration corresponds to test #50. The fuel grain is clear polymethyl methacrylate, the length is 0.305 m and the initial port diameter is 0.010 m. An alternative configuration including a post-combustion chamber has been studied, to analyze the impact of flow altering devices on performance and it corresponds to test #59. In this case, the fuel grain is blackened polymethyl methacrylate. It is shorter than the nominal configuration (0.279 m), with a Nylatron (glass filled Nylon) post-combustion chamber placed downstream of the grain (Figure 2). This post-combustion chamber has a length of 0.025 m and an inner diameter of 0.031 m. Experimental data for these configurations have been collected during tests #50 and #59 and have been post-processed through an in-house tool, see Table 1.
2. Chemistry

The combustion of PMMA includes complex chemical reactions including numerous intermediate reactions. The main product of the decomposition of PMMA is the monomer methyl methacrylate. In turn, it decomposes into combustible gaseous products. The combustion of these gaseous products leads to the formation of the final products and the release of heat. The major combustibles that are formed are methane, methanol, formaldehyde and acetylene. The possible intermediate reactions include thermal decomposition, thermal oxidative decomposition, decomposition of monomer Methyl MethAcrylate (MMA) and the combustion of methane, methanol, formaldehyde and acetylene. It is possible to distinguish a zone, in the fuel, where the temperature of the material is not affected and the material remains unchanged, as well as a heating zone where the temperature of the material increases, see Figure 3. In the heating zone, it is possible to distinguish a transition zone and a pyrolysis layer, in which not only the physical properties of the material are changed, but also the chemical composition is changed as well. The temperature at which the pyrolysis process begins is estimated to be 500 K. The transition between the pyrolysis process inside and outside the fuel grain is characterized by the surface temperature. It is defined as the temperature at which the pyrolyzing fuel is no longer in a solid state, but it is completely transformed into a gaseous state. This is estimated to occur at 700 K < Tw < 850 K.
2.1 CFD Chemical Model

The pyrolysis of the fuel needs to be simplified for the CFD model. Only the chemical process outside the fuel surface, in the gas phase, are modeled here. It is assumed that the polymeric fuel completely pyrolyzes into methane, methanol, formaldehyde and acetylene, which is released from the fuel surface and diffuses into the flame. It is not possible to directly use the ideal combustion reactions of these major gaseous products of PMMA pyrolysis as the results of simulation show a thermal behavior far from expected, with a value of temperature considerably higher than the adiabatic flame temperature. Instead, the theoretical values for the chemical process of combustion of PMMA were simulated in Chemical Equilibrium with Applications at the operating conditions of the experimental data and with a stoichiometric oxidizer to fuel ratio. With these input conditions, CEA allows the calculation of the quantities of reaction products, combustion parameters and the adiabatic flame temperature. Products of PMMA/GOX combustion with a mass fraction greater than $10^{-5}$ have been selected and a complex balanced reaction has been implemented in STAR-CCM+. It simulates the combustion of methane, methanol, formaldehyde and acetylene and gives importance to the influence of the amount of the major products of combustion on the final thermal behavior. In this case, a reduced flame temperature was observed and the overall behavior was more realistic and adherent to the real physics. The Standard Eddy Break-Up Model has been selected in STAR-CCM+ as the mechanism for predicting the chemistry. In this model, the reaction rate is modeled through an expression that takes into account the turbulent micromixing process.

The following equation is considered:

$$ ν_F F + ν_O O \rightarrow ν_{P_1} P_1 + ν_{P_2} P_2 + ... + ν_{P_j} P_j $$

where $ν$ is the stoichiometric coefficient and O, F and P are oxidizer, fuel and products, respectively. For eqn 1, the chemical reaction rate is calculated by taking the minimum of three different rates based on the mean oxidizer mass fraction, mean fuel mass fraction and the mean product mass fraction. The result is given in eqn 2.

$$ R_{F, mix} = - \frac{ρ}{M_F} \left( \frac{1}{τ_R} \right) \tilde{A} \min \left[ \tilde{Y}_F \cdot \frac{\tilde{Y}_O}{s_O} \cdot \tilde{B} \left( \frac{\tilde{Y}_O}{s_O} + \frac{\tilde{Y}_{P_1}}{s_{P_1}} + \frac{\tilde{Y}_{P_2}}{s_{P_2}} + ... + \frac{\tilde{Y}_{P_j}}{s_{P_j}} \right) \right] s_O = \frac{ν_O M_O}{ν_F M_F}, s_{P_i} = |ν_{P_i}| M_{P_i} ν_F M_F $$

The time scale $τ_R$ is the ratio between the turbulent kinetic energy and its dissipation rate, $M$ is the molecular weight, $ρ$ is the density, $\tilde{A}$ and $\tilde{B}$ are model parameters and $\tilde{Y}$ is the mass fraction. Mass fractions of fuel and oxidizer injected in the combustion chamber are user input and were set in accordance with experimental results. Individual species in the global reaction are assumed to be transported at different rates and evolve by means of individual transport equations, each with their own diffusivities. The concentration of the limiting reactant is used to determine a mass fraction scale when calculating the reactant consumption rate. This is the meaning of the operator $\min$ in eqn. 2. The integrated micromixing rate is proportional to the mean (macroscopic) concentration of the limiting reactant divided by the time scale of the large eddies.

3. CFD Hybrid Rocket Motor Model

The fluid working volume has been extracted from the internal solid surfaces for each analyzed configuration, see Figure 4. It changes with time to simulate the fuel regression as it burns away.
In the simulated model, the gaseous oxidizer flows inside the combustion chamber through an inlet (left) and the gaseous fuel is introduced along the fuel surface. Four different boundary conditions have been defined:

- **Mass Flow Inlet**: the gaseous oxidizer is introduced from the left inlet. Mass flow rate and species mass fraction are inputs for the simulation.
- **Wall + Species Source**: the fuel surface has been simulated through a no-slip condition at the wall. Temperature and species mass fractions are inputs at the wall.
- **Wall**: a no-slip adiabatic wall is assumed as the interface between the fluid working volume and the post-combustion chamber and the nozzle. (areas to the right of the white fuel grain)
- **Pressure Outlet**: values of pressure, species mass fractions and temperature have been defined as field function.

Inputs for the simulation and initial conditions have been set in accordance to experimental data, see Table 1. The initial value of fuel surface temperature has been set to 800 K, in accordance with Ref. 9. The other required parameters (such as the turbulence length scale required by the $k-\varepsilon$ model, which will be described in the next section) were defined as field function. The regression of the fuel surface has been modeled through an incremental displacement with respect to a cylindrical coordinate system. A constant user specified function has been defined to account for differences in the experimental regression rate from the theoretical regression rate. A damping factor has been applied to walls in direct contact with the fuel surface after an iterative process. It allows the movement of boundary vertices in the plane of the wall, to follow the regression of the fuel surface.

### 3.1 CFD Model Set-Up in STAR-CCM+

A three dimensional study of internal fluxes has been conducted in STAR-CCM+. A reaction regime has been set and the Standard Eddy Break-Up Model has been selected as the reacting species transport model, see subsection 2.1. It solves individual transport equations for the mean species concentrations on the computational grid. Reaction rates used in the transport equations are calculated as functions of the mean species concentrations and turbulence characteristics. A mean enthalpy equation is solved in addition to the species transport equations. The mean temperature and density are then calculated, knowing the mean enthalpy and species concentrations.

The Coupled Flow model has been selected to solve the conservation equations for mass, momentum, and energy simultaneously using a pseudo-time-marching approach. It allows the analysis of flow categories involved in a hybrid rocket combustion process: incompressible, compressible, transonic and supersonic regimes. An advantage of this formulation is its robustness for solving flows with dominant source terms such is the case here. Another advantage of the coupled solver is that the convergence rate does not deteriorate as the mesh is refined. The Courant Friedrichs Lewy number (CFL) controls the size of the local time-steps that are used in the time-marching procedure. The default value of the CFL number for unsteady flows or steady flows are not optimal in all cases. Solving the governing, discretized equations implicitly in pseudo-time results in a wider stability margin; this approach permits CFL numbers greater than unity. The large resulting local pseudo-time steps provide relatively fast convergence rates. The penalty for this approach, however, is a larger storage requirement than the explicit spatial integration scheme.\(^9\) A low CFL value has been set for the start of the combustion process. To ensure stability of the solver during the entire simulation, a linear ramp has been set to increase the CFL number based on iteration count.

An unsteady CFD analysis, including a fuel surface regression model (see subsection 3.2), has been implemented in STAR-CCM+ to capture transient phenomena. In the Implicit Unsteady approach, each physical time-step involves some number of inner iterations to converge the solution for that given instant of time. The number of inner iterations per physical time-step is harder to quantify. Generally, it is determined by observing the effect that it has on results. This number of iterations within each timestep is checked to ensure that convergence of all properties is achieved. There is an optimal balance of time-step size and number of inner iterations for each problem and desired transient accuracy.

The Reynolds Average Navier-Stokes $k-\varepsilon$ model has been selected, since it is generally well suited to applications that contain complex recirculation, with or without heat transfer, and it is a good compromise between robustness and accuracy. The realizable two-layer approach and the Wolfstein model have been adopted in the present work. The two-layer approach allows the $k-\varepsilon$ model to be applied in the viscous-affected layer.

A mesh study has been conducted and a mesh refinement has been applied, to fully capture phenomena under evaluation while minimizing computational costs. A prism layer mesh model has been coupled to the core volume mesh to generate orthogonal prismatic cells next to wall surfaces. This layer of cells improves the accuracy of the flow solution near the wall and helps to capture the boundary layer, turbulence effects, and heat transfer near wall boundaries. The number of prism layers, the prism layer total thickness, the prism layer stretching, the maximum core prism transition ratio and the volume growth rate have been selected after an iterative process.
3.2 Fuel surface regression modeling

The consumption of the fuel has been simulated through an expansion of the internal working volume. This is accomplished through mesh morphing, which allows mesh vertices to be redistributed in response to the movement of control points. The fuel surface regression is simulated through a specified time dependent function that reproduces experimental results of Table 1. The mesh morpher displacements associated with the movement of control points generate an interpolation field throughout the region which can then be used to displace the actual vertices of the mesh. Each control point has an associated distance vector which specifies the displacement of the point within a single time-step. An automatic thinning algorithm is provided; it uses an estimated deformation of the mesh to reduce the number of control vertices. All regions that are associated with this motion are morphed at the same time. The interactions between boundaries and morphing process are important to setting up a simulation for morphing. The morpher uses boundary vertices as control points for the selected boundary conditions:

- **Displacement**: the boundary vertices are moved by a specified distance. Linear displacement of boundary vertices relative to the vertex positions of the previous time-step. This morpher specification has been set for the fuel surface.
- **Constrained**: in this case, boundary vertices can move on the boundary, but they remain in the plane of the boundary. This boundary condition has been applied to surfaces in contact with the fuel surface.
- **Fixed**: mesh vertices lying on a fixed boundary plane are not moved in response to the interpolation field calculated by the morpher. This boundary condition has been applied to all the other surfaces.

4. Chemical Model Validation

The unsteady combustion process has been simulated in STAR-CCM+. The combustion chamber has been modeled as a cylinder and fuel and oxidizer have been introduced from the lateral surface and the base of the cylinder, respectively. The morphing movement, described in subsection 3.2, has also been implemented. The regression of the fuel is implemented as a function of time and is converted in an incremental displacement of boundary vertices. The initial and final diameters are matched to experimental results of test #50 (nominal configuration). The combustion of PMMA/GO2 has also been simulated in CEA at conditions of the reference test. Input for the analysis are mean pressure, oxidizer to fuel ratio, mole fractions and temperature of reactants. Table 2 compares results obtained with CEA and STAR-CCM+ after 1 second of combustion. The STAR-CCM+ EBU species mole fractions are maximum values in the flame zone. \( \text{CO}_2 \) and \( \text{H}_2\text{O} \) EBU mole fractions are near values obtained with CEA, \( \text{H} \) and \( \text{O} \) are slowly higher, while \( \text{OH} \) and \( \text{CO} \) are slowly lower, see Figure 5 for the STAR-CCM+ results. Results for major species compare favorably, giving confidence in the adopted STAR-CCM+ model. Note that we could not expect the results to match perfectly, since the EBU only uses a single step reaction.

![Figure 5: Mole fractions of O2 and CO2 from STAR CCM+ Standard Eddy Break-Up Model. Fuel aft section after 1 second of combustion.](image-url)
Table 2: Comparison of PMMA/O2 combustion results from CEA and STAR-CCM+.

<table>
<thead>
<tr>
<th></th>
<th>CEA</th>
<th>EBU</th>
</tr>
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<tbody>
<tr>
<td>OF</td>
<td>1.665</td>
<td>1.665</td>
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<tr>
<td>$p_c$ [MPa]</td>
<td>1.379</td>
<td>1.379</td>
</tr>
<tr>
<td>$t = 1s$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$T_c$ [K]</td>
<td>3360</td>
<td>3253 †</td>
</tr>
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</table>

Mole Fractions

<table>
<thead>
<tr>
<th></th>
<th>CEA</th>
<th>EBU</th>
</tr>
</thead>
<tbody>
<tr>
<td>$H_2O$</td>
<td>0.29529</td>
<td>0.29049</td>
</tr>
<tr>
<td>$CO_2$</td>
<td>0.21913</td>
<td>0.21234</td>
</tr>
<tr>
<td>$CO$</td>
<td>0.26647</td>
<td>0.20181</td>
</tr>
<tr>
<td>$H$</td>
<td>0.02416</td>
<td>0.03663</td>
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<tr>
<td>$H_2$</td>
<td>0.04454</td>
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<tr>
<td>$O$</td>
<td>0.02165</td>
<td>0.04515</td>
</tr>
<tr>
<td>$OH$</td>
<td>0.07303</td>
<td>0.04523</td>
</tr>
<tr>
<td>$O_2$</td>
<td>0.05560</td>
<td>0.05557</td>
</tr>
</tbody>
</table>

• Chemical Equilibrium with Application.
* Standard Eddy Break-Up Model in STAR-CCM+.
† Maximum value.

Figure 6 shows the temperature trends from STAR-CCM+ after 1 second and after 20 seconds of combustion simulated with the Standard Eddy Break-Up Model. Comparison of these results with table 2 show that heat released and flame temperature are in the range of the value predicted from CEA.

Figure 6: Temperature trends from STAR-CCM+ Standard Eddy Break-Up Model after 1 second (right) and after 20 seconds (left) of combustion at the aft end of the fuel grain. The port cross sections are to scale as modeled by the morphing model.

Temperature, velocity and density profiles in three axial stations are reported in Figure 7. Note that the origin of the reference system is front of the fuel and the axial coordinate ($z$) grows towards the aft of the fuel. Qualitative temperature and velocity trends are coherent with those expected from physics; a peak of temperature and velocity is registered in the flame zone, while the density is minimum. Furthermore, the average temperature and velocity increase in the axial direction, while density decreases.

Figure 7: Temperature profiles along the axial direction at three different stations.
5. Boundary layer: comparison to theory

This section compares computation of the turbulent boundary layer height above the solid fuel grain at the selected test conditions to theory in order to validate the model. According to classical hybrid combustion theory, the turbulent boundary layer is divided into two regions by the presence of a flame at a finite distance from the regressing surface. Convection and diffusion mechanisms in the boundary layer transport the fuel from the wall and the oxidizer from the free stream toward the middle of the layer and the flame is established at a point where the oxidizer to fuel (OF) ratio supports combustion. The fuel flux into the flame can be obtained from an integration of the fuel species continuity equation over the region between the surface and the flame. The oxidizer flux into the flame can be obtained from a similar integration over the region between the flame and the boundary layer edge. The rates of fuel and oxidizer entering the flame are then equated through the local ratio.

The theoretical boundary layer thickness has been calculated through the formula suggested by Marxman.\(^{15}\) It has been predicted to be a function of the blowing parameter \(B\), the free-stream unit Reynolds number, \(Re_z\), and the axial coordinate \(z\), see eqn. 3. The blowing parameter accounts for convective heat flux to the fuel surface in the presence of wall blowing. It can be interpreted as the ratio of the thermal energy of the main stream relative to the surface, to the thermal energy required to pyrolyze a unit mass of fuel. The blowing parameter can be expressed as a function of the velocity ratio at the flame \(u_e/u_b\) and the chemical parameter \(\Delta h/h_v\). In eqn. 4 the radiative heat transfer is neglected and only convective heat transfer is considered. This assumption is widely adopted for non-metalized hybrid fuels, like the PMMA being considered here.

\[
\delta = z \left[ \frac{0.0281(1 + B)\ln(1 + B)}{IB} \right]^{0.8} \quad Re_z^{-0.2} , I = \frac{7(1 + 1.3B + 0.364B^2)}{72(1 + 0.5B)^2} \quad (3)
\]

\[
B = \frac{u_e \Delta h}{u_b h_v} \quad (4)
\]

The velocity ratio at the flame can be expressed in terms of the oxidizer to fuel ratio, the chemical parameter of the system \(\Delta h/h_v\) and the concentration of oxidizer in the free stream \(K_{OX}\). The value of \(K_{OX}\) is equal to 1, since the oxidizer is pure O2, the OF value and the free-stream unit Reynolds number are assumed to be the average test #50 conditions.
as provided in table 1. The chemical parameter $\frac{\Delta h}{h_v}$ represents the ratio amidst the enthalpy difference between the flame and the wall $\Delta h$ and the effective heat of gasification $h_v$. It has been evaluated using methods outlined in the appendix of Ref. 15. The expression is:

$$u_r = \frac{u_b}{u_b} = \frac{OF \Delta h}{h_v} K_{OX} + (OF + K_{OX}) \Delta h/h_v$$

(5)

The value of the blowing parameter, calculated with the conditions reported above, is $B = 9.4$.

Figure 8a shows the boundary layer above the fuel grain at the beginning (top) and at the end of the burn (bottom). In figure 8b, blue and black curves represent the boundary layer height at the end and at the beginning of the burn; red and orange curves the flame location at the end and the beginning of the burn. Here it is assumed that the location of the edge of the thermal boundary layer corresponds to the edge of the momentum boundary layer, consistent with Ref. 13. The green curve represents the theoretical boundary layer thickness from Eq. 3 using the calculated $B$. Boundary layer and flame profiles are in accordance with experimental observation. The boundary layer thickness at the end of the burn exceed the steady state value predicted from Marxman theory, as expected from other experimental investigations.\textsuperscript{10, 20}

6. Thermal Analysis Validation

In the classical heat transfer theory for hybrid rocket, the fuel is vaporized by convective and radiative heat transfers from the flame sheet to the fuel surface. A simplified heat transfer model is reported in figure 9.\textsuperscript{21}

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{heat_transfer_model.png}
\caption{Heat transfer model. Adapted from Ref. 21.}
\end{figure}

It is assumed that all chemical reactions occurs in a thin flame zone defined as flame sheet and kinetic effects at the fuel surface are neglected. The total heat flux provided to the fuel surface take into account radiation from gas-phase products and convection. The radiative heat transfer is usually small compared to the convective heat transfer. The basic model considers that the surface responds to the heat flux instantaneously by decomposing to yield gases. The total
steady-state heat flux, $\dot{Q}$, can be evaluated through the model proposed by Marxman et al.\(^\text{18}\) It takes into account the coupling effect between radiant flux, $\dot{Q}_{\text{rad}}$, and convective heat, $\dot{Q}_{\text{conv}}$, (see eqn. 6). The radiant flux enhances the blocking effect due to blowing, whereby the vaporized fuel leaving the fuel surface decreases convective heat transfer to the surface.

\[
\dot{Q} = \dot{Q}_{\text{conv}} \left[ \left( \frac{\dot{Q}_{\text{rad}}}{\dot{Q}_{\text{conv}}} \right) + e^{-\frac{\dot{Q}_{\text{rad}}}{\dot{Q}_{\text{conv}}}} \right]
\] (6)

The total heat flux provided to the fuel surface when PMMA/O2 combustion occurs has been evaluated in a parallel thermal study at JPL.\(^\text{7}\) It is estimated to be $\dot{Q} = 1.0175 \times 10^6$ W/m\(^2\).\(^\text{7}\)

CFD analysis predicts a value of heat flux at the fuel surface of the same order of magnitude of the steady-state value, in the range $3.994 \times 10^5$ W/m\(^2\) < $\dot{Q}$ < $4.649 \times 10^6$ W/m\(^2\) as can be seen in Figure 10.

![Figure 10: Boundary heat flux from STAR-CCM+ after 1 second of combustion, internal cylinder front view.](image)

### 7. Motor Design and CFD Results

The purpose of this CFD analysis is to inform and improve the motor design. Classical hybrid rocket combustion is typically characterized by low regression rates and depending on the design, can suffer from poor combustion efficiency. The low regression rate is a consequence of the blocking effect that limits the heat transfer to the fuel wall. For small scale systems, such as that considered here, low regression rates are not a problem. The efficiency is limited by the amount of mixing in the turbulent boundary layer. A possible way to improve performance is to introduce mixing devices, to increase the amount of mixing and the residence time within the combustion chamber, which this analysis can capture.

The ratio of the length to diameter of the fuel grain is a parameter that particularly affects the combustion efficiency in the absence of a mixing device. If fuel grains are too short, there is not sufficient length for the boundary layer to develop and this typically results in the expulsion of unburned oxidizer and therefore, low efficiency. The converse is true if fuel grains are too long. In this latter case, it results in unburned fuel exiting the combustion chamber and again low combustion efficiency.

A CFD investigation of effects on performance due to the addition of a post-combustion has been conducted, to analyze physical phenomena involved in mixing process that are responsible for changes in combustion efficiency, to investigate the behavior of the internal fluxes and to inform the final design of the hybrid motor. The chemical model explained in section 2 and the computational fluid dynamics model explained in section 3 have been adopted and results are reported here.

#### 7.1 Design

The nominal configuration has a convergent-divergent nozzle right after the fuel grain. The configuration with post-combustion chamber has a fuel grain shorter than the previous configuration and the post-combustion chamber has been added after it. Table 3 displays the geometric parameters for both configurations. Four stations have been considered along the fuel length, in correspondence of the fuel front section (1), the fuel aft section (2), the throat section (3) and the exit area (4) (see Figure 11).
Table 3: Geometric parameters.

<table>
<thead>
<tr>
<th></th>
<th>Test #50</th>
<th>Test #59</th>
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<tr>
<td></td>
<td>Nominal Configuration</td>
<td>Configuration with pcc$^*$</td>
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<tr>
<td>$L_{fuel}$ [m]$^†$</td>
<td>0.305</td>
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</tr>
<tr>
<td>$L_{pcc}$ [m]$^†$</td>
<td>-</td>
<td>0.025</td>
</tr>
<tr>
<td>$D_{pcc}$ [m]$^†$</td>
<td>-</td>
<td>0.032</td>
</tr>
<tr>
<td>$L_{fuel}/D_{f}$º</td>
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<td>27.060</td>
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<tr>
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<td>0.312</td>
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<tr>
<td>$A_{3}/A_{4}$</td>
<td>0.249</td>
<td>0.251</td>
</tr>
</tbody>
</table>

$^{†}$ pcc: post-combustion chamber.

$^{‡}$ $L$: fuel length.

$^{‡}$ $D$: fuel diameter.

$^*$ $A$: cross section area.

7.2 Tests Performance and CFD Results

Performance of tests #50 (nominal configuration) and #59 (configuration plus post-combustion chamber) have been evaluated through an in-house tool. Inputs for the software are the oxidizer temperature and chamber pressure, from each test. Clear PMMA/gaseous oxidizer was used in test #50 (nominal configuration) and blackened polymethyl methacrylate/gaseous oxidizer and a Nylatron (glass filled Nylon) post-combustion chamber were used for test #59 (configuration with post-combustion chamber). Combustion chamber pressure profiles for the nominal configuration and the configuration with post-combustion chamber are reported in Figure 12. The large pressure spike observed near shutdown for test #50 is due to the purge gas starting. The chamber pressure increases during the burn and this phenomenon is still not well understood. $^{17}$ The regulated oxidizer pressure does not increase during the test resulting in a constant oxidizer mass flow. The increase in pressure can be due to a decrease in nozzle throat area due to thermal effects or, more likely, an increase in fuel mass flow.

Figure 12: Unfiltered chamber pressure data. Left: test #50. (nominal configuration) Right: test #59. (configuration with post-combustion chamber)
The regression rate has been evaluated with the theoretical formula:
\[
\dot{r} = aG_{ox}^n
\]  \hspace{0.5cm} (7)

Both \( a \) and \( n \) are empirically derived constants. For these tests, the value of \( n \) is held fixed (\( n_{lit} = 0.62 \)), the constant \( a \) is an empirically determined to match the regression observed in the test. The values of \( a \) for tests #50 and #59 are higher than the theoretical value (\( a_{lit}^{lit} = 2.11 \times 10^{-05} \)) which corresponds to a significantly higher regression rate for both configurations (see table 4). This phenomenon is believed to be caused by a mechanical break-up of the fuel under the thermal and pressure loads.\(^7\) The fuel escaping the surface during combustion appears to not completely be vaporized in test #50 and bright streaks are visible in the plume possibly signifying the expulsion of partially burned pieces of fuel. Test #59 results in better overall performance and a higher efficiency as displayed in table 4.

The efficiency of a motor is calculated with the following formula\(^2\):
\[
\eta = \frac{p_t A_{t} \dot{m}}{C_{\text{ideal}}}
\]  \hspace{0.5cm} (8)

where \( p_t \) is the total chamber pressure at station 2 (see Figure 11), \( A_t \) is the throat area, \( \dot{m} \) is the mass flow rate and \( C_{\text{ideal}} \) is the ideal characteristic velocity. The value of \( p_t \) was assumed to be equal to the mean chamber pressure measured from pressure transducers (see Figure 1), since the velocity is very low at the fore end cap. The value of \( C_{\text{ideal}} \) was determined using the thermochemical calculator CEA.

Table 4: Performance of tests #50 and #59. Data is taken from Ref. 8.

<table>
<thead>
<tr>
<th>Test #50</th>
<th>Test #59</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nominal Configuration</td>
<td>Configuration with post-combustion chamber</td>
</tr>
<tr>
<td>( a/\dot{a}_{lit} )</td>
<td>1.83</td>
</tr>
<tr>
<td>( \dot{r} [\text{mm/s}] )</td>
<td>0.477</td>
</tr>
<tr>
<td>( p_c [\text{MPa}]^\dagger )</td>
<td>1.379</td>
</tr>
<tr>
<td>( \eta )</td>
<td>0.81</td>
</tr>
</tbody>
</table>

\(^1\) pcc: post-combustion chamber  
\(^*\) lit: literature  
\(^\dagger\) Mean chamber pressure.

A CFD investigation has been conducted, to analyze physical phenomena involved in the mixing process, to investigate the behavior of the internal fluxes and the heat released during the combustion process with the goal of determining how to optimize the internal geometry for performance. An unsteady analysis was implemented and the fuel surface regression model explained in section 3.2 was adopted to capture transient phenomena and compare CFD results with experimental data. Inputs for the simulation and initial conditions were set in accordance to experimental data of test #59. A no-slip adiabatic condition was selected for the post-combustion chamber boundary in the CFD analysis. A post-combustion chamber in Nylatron was adopted in test #59, for its insulating properties. The consumption of the material during the combustion was not simulated and a fixed diameter equal to those measured after test #59 was set. The difference between initial and final diameters is less than 5\% and a stationary condition for this wall is reasonable. The model explained in section 3.2 can be adopted for this surface in future analysis.

The section enlargement at the fuel grain exit introduces a rearward step, thereby enhancing mixing. The post-chamber volume also provides the mixture more time to fully combust prior to entering the nozzle, see Figure 13. The shape of the post-chamber must be optimized in order to have a good residence time, without affecting too much the flow total pressure and engine weight.

The mean value of scalar quantities at each motor station (spatial average) has been taken into account for the following consideration. The combustion efficiency was calculated with eqn. 8, in which the mean spatial and temporal total pressure at station 2 (see Figure 11) resulting from CFD simulation was considered. Table 5 compares the value of efficiency resulting from CFD analysis with those calculated with experimental data.

The mean spatial and temporal temperature of the flow along the motor length for the configuration with post-combustion chamber is reported in Figure 14. The temperature trend is compared with those predicted for the nominal configuration. As can be observed, a peak of temperature is reached inside the post-combustion chamber.

Temperature trends for the configuration with post-combustion chamber after 1 second and 20 seconds of combustion are reported in Figure 15.
Figure 13: Mass Fractions after 1 second of combustion, post-combustion chamber cross section, front view. Left: Mass Fraction of \( CH_4 \). Right: Mass Fraction of \( CO_2 \).

Table 5: CFD efficiency comparison to performance of test #59.

<table>
<thead>
<tr>
<th>Test #59</th>
<th>CFD</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \eta )</td>
<td>0.84</td>
</tr>
</tbody>
</table>

Figure 14: Temperature trend along the motor length.

Figure 15: Temperature trend, post-combustion chamber cross section, aft view. Top: After 1 second of combustion. Bottom: After 20 seconds of combustion.

8. Future works

A hybrid rocket motor including mixing devices can give an efficiency higher than the configuration of the basic motor. On the other hand, the local motor wall is reached by hot combustion gases, therefore insulation must be increased for
longer burns. Advantages and disadvantages have to be taken into account to select a suitable configuration. A system study trading increased mass of insulation with increased efficiency needs to be conducted. Effects of the addition of a diaphragm are currently being studied at NASA-Jet Propulsion Laboratory. This device may enhance the mixing of species and therefore the combustion efficiency, however it will also introduce weight to the system. Further tests and analysis will be carried out and CFD simulation results will be used to inform the final design.

9. Conclusion

A CFD analysis has been conducted to investigate the behavior of internal fluxes during the combustion process and determining the effect of new flow altering devices in an attempt to improve performance.

An unsteady combustion model has been implemented and PMMA/GOX combustion has been simulated. The combustion model was validated and applied to model the internal fluid dynamics of two reference tests. Results of an internal fluid dynamics study for a configuration with post-combustion chamber are reported here. It was observed through the CFD results that the addition of a post-combustion chamber enables more complete burning of the combustion products before they are expelled through the nozzle. The effect of the post-combustion chamber is an increase of the mixing of the chemical species participating in the combustion process, since re-circulation of species take place inside the post-combustion chamber. Better performance and a higher efficiency have been observed by including this post-combustion chamber. However, the benefits of this addition may be outweighed by the increased mass of the insulation required and further studies are required.

10. Acknowledgements

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