Development of a Multidisciplinary Framework for Hybrid Rockets

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Abstract

Hybrid rocket propulsion is characterised by one propellant being a liquid and the other one a solid and it is becoming increasingly popular among New Space launch vehicles. In fact, companies like HyImpulse or Gilmour Space are developing sounding rockets or even small orbital launch vehicles that use hybrid rocket motors. However, the technology is still not as developed as liquid or solid rockets are . It is known that hybrid rockets can be an environmentally friendly and cost-effective option, which could explain the recent trend to use them as the industry transitions into an ecosystem of affordable access to space. In this context, this work intends to provide a tool for the development and optimization of hybrid-propelled launch vehicle concepts, using custom, adjustable models developed in a MATLAB environment to suit a wide range of requirements and mission types. Four different disciplines – Propulsion, Sizing, Aerodynamics and Trajectory – are iterated on an MDF optimization loop. The program uses inputs from DATCOM and NASA's CEA code for the aerodynamic coefficients and for the combustion chamber thermodynamic properties, respectively. The trajectory module was upgraded to a 3-DOF with rotation model, allowing the optimization to support constraints and multi-objective function variables such as apogee and burnout velocity. These combined methods grant this tool a multidisciplinary approach that is not very common in hybrid propulsion design optimization.

The tool was validated and developed for rockets using the nitrous oxide-paraffin propellant combination, but other propellant choices are possible. The results are consistent with flight-proven rockets.

Keywords: Hybrid Propulsion, MDO, Suborbital Rocket, MATLAB, Trajectory

1. Introduction

Space travel has been a reality for more than sixty years. However, rockets and rocket-powered spaceplanes remain the only transportation vehicles capable of reaching space and achieving orbit of the Earth. Further developing rocket technology is, therefore, key in increasing accessibility to outer space.

The advancements made so far already allow many different countries and companies to place satellites in orbit for varying purposes, from military applications to space tourism and the demand for launchers is still increasing, particularly for small satellites. Small satellites can be launched individually or using some sort of rideshare solution. However, the latter is not ideal for many applications. Hence, there will always be a niche for dedicated small launchers for small payloads and they are becoming increasingly popular. This is being regarded as part of the New Space era, a significant wave of trends that are shaping the space sector into being more liberal and agile.

Environmental concerns, paramount in the 21st century, and profitability are two variables that must be considered when designing a modern launch vehicle. One common approach that addresses these issues is designing the vehicle to be cheap to mass produce and efficient. One way to accomplish this is to employ hybrid rockets as the main propulsion devices in small launch vehicles, strategy that has gained some foothold in the industry [1].

Finally, designing a rocket is necessarily a multidisciplinary endeavour, which directly correlates to the objectives of this work. A multidisciplinary optimization of the vehicle's design can not only lower the needed resources (specially, propellant) and accompanying pollutant emissions of a vehicle, but is also vital for one intended to be economically competitive.

Under this context, this work reports on the ongoing development of a software tool for the design optimization of new hybrid-propelled launch vehicle concepts, using custom, adjustable models developed in a MATLAB environment to suit a wide range of requirements and mission types. This follows the previous work and software developed by Klammer [2] and Yamada [3].

2. Hybrid Rocket Technology Background

Chemical bi-propellant rocket propulsion, the most common type of rocket propulsion, is characterised by burning two propellants - a fuel and an oxidizer - in a rocket engine. In a liquid propulsion system, the fuel and the oxidizer are stored in separate tanks before they are fed into the combustion chamber, using pressure or pumps. Conversely, in a solid rocket motor, the fuel and the oxidizer are mixed and bonded together in a solid state fuel grain which burns when ignited.

Hybrid rocket propulsion concepts, on the other hand, as the one illustrated on Figure 1, make use of these two propellants in different states of matter. One, usually the fuel, is a solid and the other, usually the oxidizer, is in liquid form. Hybrid rockets are a blend of their solid and liquid counterparts not only in relation to the propellants themselves, but also in the techniques and technology used.

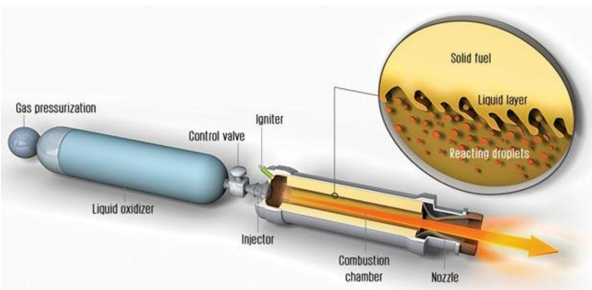

Figure 1: Schematic of a Hybrid Rocket Engine. This example features a pressurizing gas tank. Source: [4].

2.1. Similarities to solid propulsion

Hybrid rocket engines (HRE) feature a solid "block" of fuel, called grain, stored inside the combustion chamber, much like a solid rocket motor (SRM). A SRM can be made without moving parts and that can help explain why they are considered relatively simple machines. The same cannot be said of HREs, which require at the very least an actuated oxidizer valve.

The most common shape for a solid rocket is a cylindrical tube containing the propellant grain which, in turn, also features a built-in hollow core. This empty core is where the combustion will take place, as the grain is consumed from its inside walls while its external surface is protected from the flame, placed against the motor's casing. The propellant grain core cross-section can be given any shape, with the simpler option being a circle. The shape is directly related to the size of the burning surface, which directly influences the pressure and thrust generated by the motor. Some examples are shown in Figure 2.

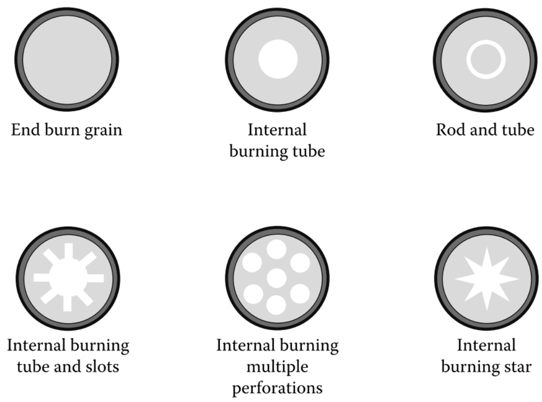

Figure 2: Six examples of propellant grain perforation configurations. Source: [5].

Hybrid rockets commonly feature two sections unprotected by the fuel grain - the pre-combustion and the aft combustion chambers, situated on the forward and aft sections of the chamber, respectively. These sections need to be protected by an insulating layer, otherwise the interior temperatures, higher than the melting point of metals, would destroy the casing [6]. Thermal insulation layers are designed to prevent casings from absorbing too much heat during motor operation.

2.2. Similarities to liquid propulsion

Processes and components of hybrid rockets similar to those found in liquid rockets include, for example, the combustion chamber injectors. These are a combination of perforations, tubes and manifolds that connect the liquid propellant feed lines to the inside of the combustion chamber. These perforations, or holes, on a bulkhead-type wall form the injector assembly, which main purpose is to mix the propellants efficiently inside the combustion chamber [5]. This is usually achieved by splitting the liquid into small droplets (atomization), making sure the gases mix in the correct stoichiometry and disperse as intended throughout the combustion chamber [7]. In the case of HREs, since there is only one liquid propellant being injected, the injector design can be simpler, as there is no mixing involved, just atomization and dispersion. The mixing happens along the length of the solid fuel grain, which sits inside the elongated combustion chamber.

Perhaps the most easily interchangeable major component between liquid and hybrid rockets is the liquid propellant tank. That propellant is usually the oxidizer in the case of hybrid motors. It is of paramount importance for the tanks to be lightweight, in order to decrease the total dry mass of the rocket. This is usually achieved by making the tanks out of materials such as aluminum, steel alloys or fiber composites. These materials are both light and strong enough to hold the pressure inside the tank. In fact, another aspect crucial for many space vehicles is the pressurized manner in which liquid propellants are stored. The reasons for this are varied and include [7]:

- In pressure-fed engines, a high-pressure propellant feed is required at the injectors and since fluids moves from high to low pressure zones, the propellant tank needs an operating pressure higher than that of the combustion chamber of the engine;
- In pump-fed engines, tank pressurization, although at lower pressures, is still important to push the liquid propellant into the pump, mitigating cavitation;
- Some propellant tanks double as structural elements of the launch vehicle and a pressurized vessel can withstand greater structural loads without deforming (the phenomenon can be observed with drink cans, which are easily crushed once opened).

Hence, the necessity of a tank pressurization system is also a commonality between liquid and hybrid propulsion systems. Some tanks are pressurized using mechanical systems such as pistons or flexible bladders, but the most common approach, at least in space applications, is to use direct gas pressurization [7].

The most common approach to tank pressurization, not only on hybrid rockets but in general, consists of using an inert gas (usually Nitrogen or Helium [7], stored in a separate tank) pressurization system. Another option relies on the use of self-pressurizing propellants and is commonly used when nitrous oxide is the oxidizer. Section 2.3 explores these propellants in greater detail.

Finally, hybrid and liquid propellant rockets share a functional upper hand over conventional solid rocket architectures which is the ability to produce variable thrust [8]. Liquid and hybrid engines can produce variable thrust in a non-prescribed random manner as needed during flight, using a feature called throttling. On HREs, this is achieved by adjusting the oxidizer valve aperture, feeding the combustion chamber injector assembly with a lower mass flow than optimal. Because thrust is almost proportional to the propellant mass flow, this actuation of the valve results in an almost proportional control of the thrust. While pressure-fed engines use valves, pump-fed engines can throttle by changing the rotary speed of the pumps [7]. This ability comes at a cost, however, since injector flow dynamics change as the overall mass flow through the engine is reduced, stripping away efficiency from atomization and mixing. All in all, when lowering the throttle in an engine to a sub-optimal mass flow, the chamber pressure and specific impulse decrease.

Also, the geometry of solid propellant grains can be tailored, during design and production, to manipulate the way the thrust varies over time and obtain specific thrust profiles. Several examples of this are shown in Figure 2.

2.3. Propellants

An analysis of the different propellants available for hybrid engines can be divided into two sections, the oxidizers and the fuels. Starting with the liquid oxidizers, right away the two most common choices are liquid oxygen (LOX) and nitrous oxide (N_2O) [6]. LOX is a well-known propellant and provides great performance overall. It's deeply cryogenic, so it is adequate for large hybrid boosters, for example, but not for use-cases requiring a storable chemical.

Nitrous oxide is a more niche propellant than LOX, with its use being more famous in hybrid rocketry than elsewhere. They share as advantages their lower toxicity and cost when compared with other oxidizers such as N_2O_4, for example, a typical storable, hypergolic propellant. Virgin Galactic's SpaceShipTwo, which propelled four passengers plus a crew of two to the edge of space (86 km in altitude, to be precise) in July 2021, uses nitrous oxide, making this probably the most high-profile use of the oxidizer on a hybrid propulsion system. On the other hand, nitrous oxide is popular among small, often times amateur, hybrid rocket engines, in part thanks to its self-pressurizing property and relatively safety. Even so, it can decompose quickly if heated or in the presence of impurities, which poses a storage risk.

The oxidizer tank sometimes does not need to be pressurized by a dedicated pressurization system, as discussed in section 2.2. This is mostly dependent on the oxidizer itself. If the oxidizer is self-pressurizing, external pressurizing equipment may not be needed. Self-pressurizing propellants are liquid substances or mixtures that evaporate in such a way that the gaseous phase provides high enough internal pressure to the propellant tank to feed the oxidizer injector (and, hence, the combustion) effectively. This is one of the advantageous properties of nitrous oxide, thanks to its high vapor pressure at room temperature of around 50 bar.

The mixture of LOX and N_2O has been studied as a viable, self-pressurizing, refrigerated oxidizer, where the more volatile LOX is dissolved in cold nitrous oxide and, as it evaporates, creates pressures of up to 120 bar, which is enough for a wide range of applications [9]. Due to the nitrous oxide being refrigerated to negative temperatures, this mixture is denser than pure N_2O but it still retains the self-pressurizing property and is less prone to decomposition.

Another common oxidizer choice is hydrogen peroxide (H_2O_2). Peroxide has a great heritage as a rocket fuel in Europe, most notably in Great Britain. The 60s British orbital launcher Black Arrow burned peroxide and RP-1 in its liquid rocket engines. Peroxide also burns adequately with solid fuels, making a very volume-efficient combination, as high concentration H_2O_2, called High-Test Peroxide (HTP), has a density almost 50% greater than water. Like nitrous oxide, it also suffers from stability issues and should be stored and handled with great care [9].

As for the fuel in a hybrid rocket motor, it corresponds generally to the solid propellant and is oftentimes considered the bottleneck when it comes to making large hybrid motors viable, due to the difficulty of getting traditional solid fuels to evaporate quickly enough to obtain relevant thrust outputs [9]. That is the case of hydroxyl-terminated polybutadiene (HTPB), a low-energy chemical frequently used in solid rocket propellants as a binder, turning an otherwise incohesive mixture of fuel and oxidizing agents into a homogeneous propellant. Alone, it can be cast into a hybrid combustion chamber and will achieve a respectable performance with various oxidizers.

Polybutadiene acrylonitrile (PBAN) has a similar role and properties to HTPB. It is being used as a constituent of the solid propellant on NASA's Space Launch System boosters and has also seen use as a hybrid fuel. According to Calabro [10], one of the highest values of specific impulse ever recorded from a hybrid engine test, around 380 seconds, used PBAN with lithium and lithium hydride as a solid fuel. The oxidizer was a mixture of liquid oxygen and liquid fluorine.

Metal additives have been added to solid fuels to try to increase its performance, either by increasing the regression rate of the fuel grain or by shifting the oxidizer to fuel ratio. Aluminum powders and metal hydrides like the lithium hydride mentioned before are common examples. 3D-printing plastics such as ABS have also been tested on small engines and are easily accessible and safe for amateurs or university laboratories. Polyethelene also saw extensive testing as a hybrid fuel by General Electric [10]. In fact, almost any combustible material can be burned in a hybrid combustion chamber and generate thrust, albeit few will give useful performance.

2.4. Increasing the regression rate

The combustion process and internal ballistics of a hybrid motor are considerably different from both solid and liquid engines [6]. For adequate burning to occur, the oxidizer and the fuel must be thoroughly mixed. In a solid motor, they are mixed before being burned. In a liquid engine, the mixing happens shortly after injection into the chamber, with the two propellants mixing as they vaporize. In a hybrid, the two propellants aren't mixed as soon as they become gaseous. The hot combustion inside the chamber heats the outer layers of the fuel grain core, causing them to evaporate, as drawn in Figure 3. This forms a film of fuel vapor covering the rest of the still solid fuel. Eventually, this boundary layer of gas mixes with the also gaseous oxidizer stream flowing through the center of the combustion chamber, from the injector. The mixing and combustion process takes place between these two layers of pure fuel and oxidizer.

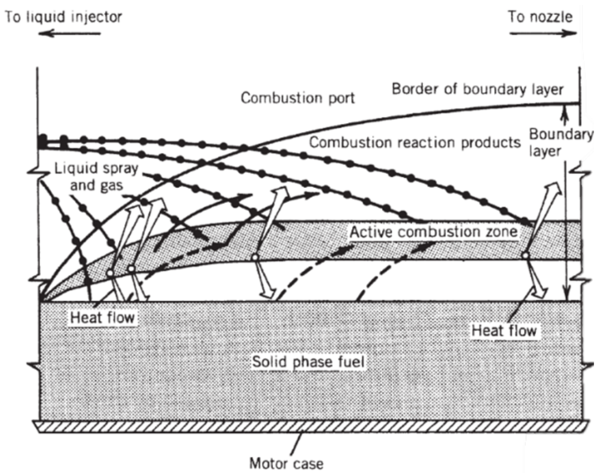

Figure 3: Illustration of the three boundary layer model of the hybrid combustion process. Source: [7].

This implies that, in a hybrid motor, heat transfer to the solid fuel is ruled by the behaviour of the boundary layer. Because of the boundary layer effect, the complete mixing and combustion of the last portion of the fuel grain only happens further downstream from the grain end - hence, an aft-combustion chamber, about as long as the chamber is wide [6], is usually needed before the nozzle to improve the combustion efficiency of the motor. This unique combustion process also has implications in the solid fuel regression rate - the rate, usually measured in mm/s, at which the solid fuel surface is consumed. As the fuel surface absorbs heat from convection and radiation, its vaporization creates the fuel boundary layer and, thus, a "blowing" effect that counters the heat transfer. Without an effective heat transfer mechanism, fuel regression rates are low and insufficient to generate the levels of thrust needed for large hybrid rocket boosters and many other applications.

Several approaches have been pursued to solve this issue, most of them intended to facilitate the heat transfer to the fuel [9]. One is called the mixed hybrid approach, wherein the solid fuel is doped with a small amount of solid oxidizer. A similar approach is to use metal additives in the fuel, as mentioned in section 2.3, to increase the heat radiation mechanism to the fuel [7]. On the other hand, the problem can be addressed by increasing the surface area of the fuel, instead of increasing the regression rate, but this does not lead to satisfactory solutions in most cases. To increase the surface area, the chamber volume also needs to be increased or a multi-port design is employed. Each option has their own disadvantages, but they both lead to a lower filling factor (empty volume) and consequent higher structural mass fraction of the rocket vehicle.

While increasing the regression rate has been historically difficult, a new class of liquefying (or "melting") fuels gained popularity in the late 1990s that could solve this issue. When heated, these fuels turn from solid to a low viscosity liquid state before being vaporized, unlike HTPB or PBAN. From this group of fuels, paraffin wax stands out as one of the most popular. Stanford University pioneered the research into paraffin at the start of the millennium. It was first fired at Stanford University in 1998 with oxygen as the oxidizer [9]. Paraffin in HREs burns at a regression rate several times higher than common polymeric fuels, thanks to a process called entrainment, in which fuel droplets from the melting surface of the fuel are released into the flow, vaporizing away from the blowing effect of the fuel boundary layer - effectively increasing the fuel mass flow rate. The dominant constraint on the regression rate ceases to be the rate of heat transfer to the fuel and becomes the viscosity and surface tension of the liquid fuel layer. Entrainment is the process represented on the magnified detail of Figure 1.

2.5. Performance and use-cases

In terms of performance, hybrids also occupy the middle space between solids and liquids, although they are much less mature and less tested. One of the better developed hybrid propellant combinations so far is liquid oxygen with HTPB fuel, which gives acceptable performance (its nominal I_{sp} of 280 seconds and low O/F ratio are comparable to the main orbital launch vehicles operating in the commercial market). However, HTPB is being dropped in favor of higher regression rate fuels, like paraffin, for high-thrust cryogenic booster stage applications.

Such is the case of HyImpulse Technologies. This start-up was formed in 2018, stemming from a research group at the DLR (German Aerospace Center), whose founders' first experience with hybrid rockets had been in student sounding rocket projects [1]. Their aim is to differentiate themselves from the rest of European small launcher start-ups by using hybrid propulsion in their vehicles. They are developing a modular three-stage small launch vehicle which they claim will be able to put 500 kg payloads into a dedicated orbit.

The rocket will use a proprietary paraffin-based fuel, to which a minor percentage of additives is added, and liquid oxygen as the oxidizer. This promises to be an environmentally friendly combination, as well as relatively easy and safe to be handled during the manufacturing process and launch operations, one of the major hurdles being the handling of liquid oxygen at cryogenic temperatures and its loading into the vehicle [11].

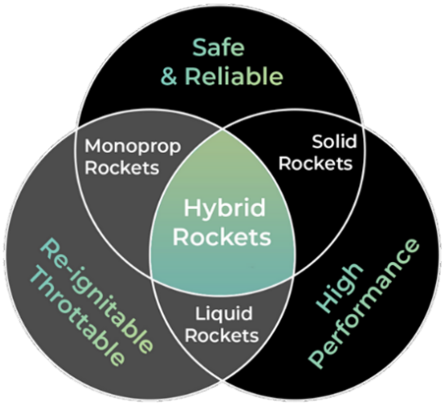

Figure 4: HyImpulse's visualisation of the combined strong points of solid and liquid propellant rockets (and monopropellant configurations as well) in hybrid rockets, as presented on their website [1].

The better performing hybrid propellant pairs are metallized fuels with fluorine oxidizers, with measured specific impulse values of up to 380 seconds, but these are expensive and/or dangerous, in many cases defeating the point of using hybrid propellants in the first place.

N2O and paraffin wax, not necessarily together, have seen a growing popularity in recent years among amateurs and universities due to the ease of handling and operation. The two together produce an I_{sp} of 248 seconds, with an oxidizer-to-fuel ratio of 8. Nitrous oxide is a particular good fit for low-mass, small sounding rockets, since the self-pressurization allows tight mass budgets to be feasible.

Figure 4 illustrates some of the advantages of hybrid propulsion, which translate to some interesting use cases, such as missions requiring throttling and restart capabilities, when safety and simplicity are more important than performance; replacing solid upper-stages and kick motors; lowering pollutant emissions by replacing solid propulsion devices which burn ammonium perchlorate.

3. Hybrid Rocket Optimization Problem Implementation

Conceptualizing a rocket vehicle is a complex design challenge that benefits from breaking down the full system into smaller, less complex parts, modelling each one separately and analyzing their interactions. In this spirit, rocket design is usually split into various interdependent subsystems, like the propulsion system, structure, aerodynamic and control surfaces, etc.

3.1. Mission requirements

There's another subsystem that deserves a mention - the payload. No transportation vehicle is made without a purpose and a rocket's goal is usually to deliver a payload to a destination. Like luggage on an automobile, the payload is not needed for the rocket to function, except when it is also playing a structural and/or aerodynamic role. However, the payload is instrumental in defining the mission requirements for a launch vehicle [12].

The capability of a rocket vehicle is usually measured in terms of how much payload mass it can place at a given altitude, at a given velocity. For orbital launch vehicles, this can translate to being capable of putting a 500 kg payload into Low Earth Orbit (LEO), as is the case with HyImpulse's SL1 rocket [1], for example. For suborbital vehicles, it can translate to reaching a given apogee (with null vertical velocity). In either situation, the payload must be accelerated to a precise velocity vector at a precise point in space (or in the atmosphere).

For the purposes of conceptual design validation and optimization, a full set of orbital elements isn't necessarily required or relevant. Thus, it is possible to model a launch vehicle's mission objective in a simplified way, using a target scalar velocity, with the appropriate flight path angle, at the target altitude at which that velocity must be verified. These three variables are, thus, constraints on the optimization algorithm being defined here.

Additionally, a commercial rocket designer and manufacturer is not interested in developing a vehicle that fulfils the mission requirements whatever the cost. The gross lift-off weight (GLOW) of the vehicle is a central variable for estimating cost and, as such, it can be minimized in the design as a simpler alternative to estimating and optimizing the cost, which is not a straightforward subject. Cost is an important factor, but environmental and operational concerns also drive the need for minimizing the mass of the vehicle. Likewise, minimizing the amount of propellant consumed directly minimizes pollutant emissions generated from using the propellant or from producing it. The best indicator of propellant consumption efficiency is the specific impulse.

Then, I_{sp} and GLOW are the two variables that constitute the multi-objective function of the optimization algorithm, which is to be minimized.

3.2. Propulsion subsystem

The hybrid propulsion system is simulated using the framework developed by Klammer [2] and Yamada [3], wherein three control volumes are modelled to represent the oxidizer tank, the combustion chamber and the nozzle. Mass and energy fluxes are simulated from the oxidizer tank, through the chamber and to the nozzle. In addition to these three components, only one other is modelled - the injector. Otherwise, the tool does not model ignition devices or cooling systems. There is also no tank pressurization system being modelled because the tool was developed under the assumption that nitrous oxide would be the oxidizer of choice, which is self-pressurizing. This does not mean the tool cannot function with other oxidizers, but some hard-coded parameters need to be changed accordingly and the user has to design an adequate pressurization system separately, if desired.

The oxidizer is stored in both liquid and gaseous phases inside the tank. Its two-phase equilibrium is modelled by a sub-function that uses a table of thermodynamic properties of the oxidizer at saturated conditions, from the melting point up to the critical temperature. This way, knowing the oxidizer vapor pressure (which corresponds to the tank pressure, p_{OT}) and the pressure loss through the injector and feed system, p_{feed}, the possibility of oxidizer flow to the combustion chamber is verified. If the combustion chamber pressure, p_{CC}, is such

$$p_{OT} - p_{feed} - p_{CC} > 0 \tag{1}$$

then the pressure in the tank is enough to sustain the oxidizer flowing to the chamber. This is quantified by the oxidizer mass flow rate, $\dot{m}_{ox}$, and calculated by means of equation 2, under the assumption of incompressible single-phase fluid flow.

$$\dot{m}_{ox} = C_{inj}\sqrt{2\rho_d(p_{OT} - p_{feed} - p_{cc})} \tag{2}$$

where C_{inj} is the effective injection area, obtained by multiplying the injector area by a discharge coefficient, and ρ_d is the discharge fluid density.

The fluid in the combustion chamber is assumed to be homogeneous, with the combustion process modelled as instantaneous and complete. To assure this is a reasonable assumption, the combustion chamber is sized so that the fuel grain sits between two empty portions of the chamber of combined length greater than the external radius of the vehicle, d_{ext} - the pre-combustion and the aft combustion chambers. They improve oxidizer atomization and combustion completeness, respectively.

One limitation of the software tool is how it only simulates cylindrical grain port shapes. This facilitates the simulation of the fuel regression, since it only depends on the regression rate as shown on Figure 5. Although this rate can vary axially along the length of the grain, the fuel is assumed to regress uniformly in the code as the uncertainty associated with modelling those differences would make the additional accuracy not be worth the added computational cost [2].

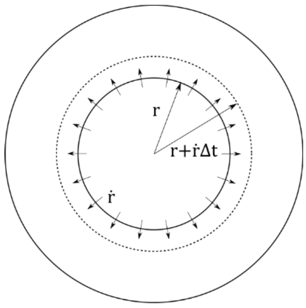

Figure 5: The fuel grain regression model implemented considers the regression rate is uniform on both the axial and the radial directions. $r = r_{port}$ is the radius of the fuel port, while $\dot{r}$ is the regression rate of the fuel surface. Source: [2].

Usually, in the literature [7], the fuel regression rate is given by

$$\dot{r} = aG_{ox}^{n} \tag{3}$$

where a and n are empirically-fitted parameters highly dependent on the propellant choices and G_{ox} is the oxidizer mass flux through the port, obtained iteratively by dividing the oxidizer mass flow rate by the port section area, which gradually increases as the fuel is consumed. The fuel mass flow rate, $\dot{m}_f$ is also given iteratively by multiplying the fuel port surface area by the regression rate and the fuel density:

$$\dot{m}_f = 2\pi r_{port} L_f \dot{r} \rho_f \tag{4}$$

As explained by Klammer [2], the regression rate's a and n empirical parameters originally used in the simulation tool were determined considering the full average mass flux through the port, G (calculated including $\dot{m}_f$), in the equation instead of G_{ox}, so that is still implemented and parameters are set accordingly. It is fairly simple to switch the code to use the oxidizer flux only, if necessary.

The oxidizer mass flow rate, $\dot{m}_{ox}$, is one of the most relevant parameters in hybrid rocketry, because G_{ox} depends on it and fuel flow, in turn, depends on G_{ox}. As explained in section 2.2, this allows the thrust of a hybrid rocket to be controlled by limiting oxidizer flow by means of a valve, for example. Although this feature is not modelled in the present work, it is something that could be added in the future.

Finally, the flow behaviour in the nozzle section is simulated using ideal nozzle theory, under the assumption of isentropic, ideal gas flow. The nozzle's throat diameter and area ratio are design variables supplied by the optimizer. The combustion chamber pressure and the oxidizer-to-fuel ratio are used as inputs to search for the other corresponding chamber properties in look-up tables, which data is compiled from NASA's Chemical Equilibrium with Applications (CEA) program [13] for the appropriate propellant combination. CEA does not have many of the hybrid propellants on its default library, but they can be manually introduced if their composition and formation enthalpy are known.

3.3. Trajectory and Control

Klammer [2] and Yamada [3] have previously included in their hybrid rocket optimization codes a 1-degree of freedom (DOF) trajectory simulation function, first developed in 2016 by Michael Pearson [2]. However, when the scope of this work was defined, it became clear that a 1-DOF model would soon be insufficient as the program evolves. Hence, developing a new three-dimensional model was made a priority.

Section 3.1 explored how the mission requirements under consideration for the purposes of booster stage and sounding rocket conceptual design optimization are the payload mass, the apogee (or booster separation altitude), and the velocity vector, $\boldsymbol{v}$ - or, simpler still, the speed, v, and the flight path angle, γ, which is illustrated on Figure 6 and defined as

$$\gamma = \arctan \frac{\dot{z}}{\dot{x}} \tag{5}$$

where $\dot{x}$ and $\dot{z}$ are, respectively, the horizontal and vertical components of the velocity vector [14].

In fact, the new 3-DOF trajectory discipline provides the needed outputs to optimize a vehicle for those mission requirements. The payload mass is a design parameter, while the vehicle's position and velocity vectors as a function of time, in cartesian coordinates, are calculated and placed in the state structure of the simulation program to be passed along to other functions. As inputs, the trajectory module needs, besides the design variables and general program parameters, the thrust and propellant mass data as a function of time, the launch altitude and angle, and general geometric and mass values for the computation of aerodynamic forces and moments of inertia.

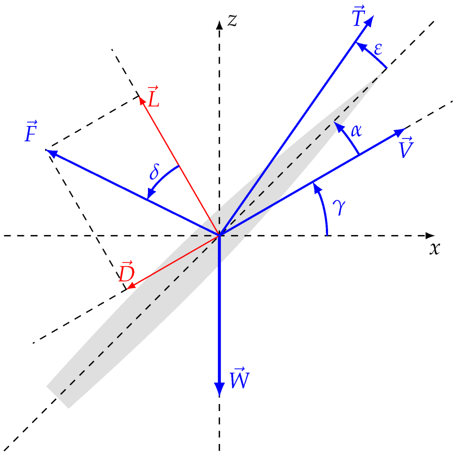

Figure 6: A diagram of a rocket flying in the positive x and z directions. The forces acting on the vehicle are shown (thrust, $\boldsymbol{T}$, weight, $\boldsymbol{W}$, aerodynamic force, $\boldsymbol{F}$) as well as its velocity vector, $\boldsymbol{v}$, angle of attack α, flight path angle, γ, and thrust vectoring angle, ϵ. $\boldsymbol{F}$ is split between its two components, drag and lift, illustrated in red. Source: [14].

The vehicle's motion variables are computed on a *while* loop. At the end of each iteration, the variables are stored, and the simulation time is incremented. The loop breaks when the vehicle returns to ground altitude, after following a ballistic trajectory from wherever propulsion ceased.

The vehicle altitude $z(t)$ is used at each time step to calculate atmospheric properties, namely air pressure, density and local speed of sound, through the 1976 COESA model MATLAB function. The model is extrapolated up to an altitude of 150 km, above which the program considers a vacuum. Likewise, the altitude, Mach number and angle of attack are used to search for the corresponding lift and drag coefficients, C_L and C_D, from look-up tables estimated for a sounding rocket by the Digital DATCOM script, an implementation of the United States Air Force DATCOM [15].

The following phase is the pitch guidance, which relevance is dependent on the type of vehicle and mission. A sounding rocket should not require pitch guidance, nor is it likely to have thrust vectoring control (TVC) or aerodynamic control surfaces to follow any active guidance. But for orbital-class vehicles, an adequate trajectory profile, usually called a gravity turn, is an optimum way of reaching the desired altitudes and speeds. For these vehicles, until the propulsion system cuts-off, a guidance algorithm is run to determine the desired pitch, θ_d, for the vehicle.

This is achieved in three phases. First, once the vehicle clears the launch tower, θ_d is increased linearly, with the linear rate being handled by the optimizer. Then, after a certain time, the desired pitch decreases exponentially, to allow for a smooth transition into the third phase, the gravity turn itself, during which the pitch guidance law is simply $\theta_d = \gamma$.

θ_d is then introduced as a reference into a simple proportional feedback controller, where it is subtracted by the simulated pitch angle, θ, obtained from the dynamics equations in the previous time step. This difference is multiplied by a simple negative gain, ranging from 0 to -1, to obtain ϵ, the TVC angle. This goes through a saturation condition to ensure it does not exceed the maximum allowed TVC angle magnitude, which is a simulation parameter.

Finally, the equations of motion, through which the accelerations in x and z are calculated, are adapted from Equations (21a-b) of Campos and Gil [14].

3.4. Numerical Methods

Throughout the MATLAB program, but especially in the Propulsion and Trajectory disciplines, some numerical approximations must be done. At each time step in the Trajectory and Propulsion function loops, ordinary differential equations are integrated using the Forward Euler method, an explicit first-order Runge-Kutta algorithm. The error of this method is proportional to the step size, so a compromise between speed and accuracy has to be arranged. The time step size, Δt, is an easily changeable parameter in the program.

As an example, the horizontal position, x, of the vehicle is determined, at each time step i, by using the Euler method such that

$$x(i+1) = x(i) + \dot{x}(i)h \tag{6}$$

where h is the step size, which is a fixed discipline parameter.

Linear interpolation is used to extract values from the look-up tables for the N_2O saturation and CEA combustion chamber thermodynamic properties. Cubic spline interpolation is used on the trajectory discipline to get continuous thrust data. For the aerodynamic force coefficients, no interpolation is done. Rather, the nearest value is chosen to impede small numerical variations in the angle of attack to introduce a lift component on the vehicle. The root-finding bisection algorithm is employed to determine the temperature of the oxidizer tank and the Mach number of the nozzle flow. The secant method was previously used, but this was changed because the program would sometimes crash when the secant method tried to calculate the internal energy of a negative temperature. Using the bisection method guarantees these variables stay within bounds and converge.

4. Validation & discussion

The Propulsion system was not substantially altered since Yamada [3] analysed and validated its results against experimental data from three different small hybrid sounding rockets from the Spaceport America Cup competition, using the N_2O and paraffin-based fuel propellant combination. His simulations showed the thrust, pressure and tank temperature profiles agreed with the test data with an acceptable error for conceptual design purposes, given the uncertainties associated with the data. Table 1 shows the summary of the model errors obtained on those three comparisons with test data. Figure 7 shows the simulated thrust curve of Phoenix 1A compared to its experimental data. Table 1 and Figure 7 were extracted from [3].

Table 1: Relative errors between simulated variables and test data from three hybrid engines [3].

Rocket Name	Deliverance II	Boundless	Phoenix 1A
p_{OT} error	1.55 %	15 %	-
p_{CC} error	10.7 %	25.7 %	12.3 %
T error	7.55 %	32.8 %	12.2 %

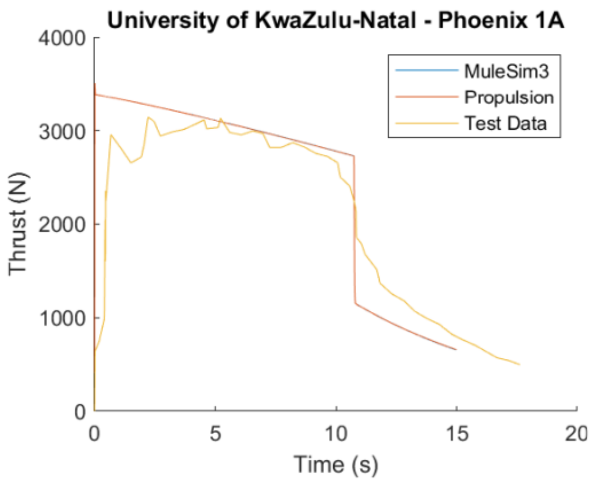

Figure 7: Comparison between the real experimental data, in yellow, and the simulated data from the hybrid rocket Propulsion function, in orange. Source: [3].

Regarding the newly developed Trajectory discipline, it was first validated by checking that the flight simulations matched the results obtained on other similar tools, such as OpenRocket, for the same inputs. The maximum error found on single variable (apogee, maximum velocity, maximum acceleration, time to apogee) comparison was 5% when testing with low-altitude sounding rocket designs. The new 3-DOF code was also compared with the former 1-DOF script on sounding rocket (up and down) flights and the errors were negligible ($\leq$1%), indicating the tool retained its accuracy in vertical flight.

Validation was performed by comparison with experimental flight data as well. By running the trajectory script with experimental thrust and inertial data from a given test-flown rocket, it is possible to compare the results obtained with the data measured in flight. Table 2 shows the comparison between experimental data recorded from the flight computer of the Xi-16 rocket, launched on February 16, 2020, by Richard Nakka [16] and the corresponding simulated flight. Some uncertainties can help explain part of the error. The thrust curve of the engine corresponded to static test fire data, not from the flight itself. There is no guarantee the solid rocket motor from Xi-16 performed equally on both occasions. Additionally, the aerodynamic coefficients were estimated, using DATCOM, for another rocket, similar enough in shape and size so as the resulting coefficients to be similar, but certainly not identical.

Table 2: Relative errors between simulated flight and test flight data from the Xi-16 flight.

Variable	Apogee	Maximum Acceleration	Time to Apogee
MATLAB tool	1034 m	185 m/s^2	14.15 s
Xi-16 flight	1150 m	220 m/s^2	14.3 s
Relative error	10.1 %	15.9 %	1.1 %

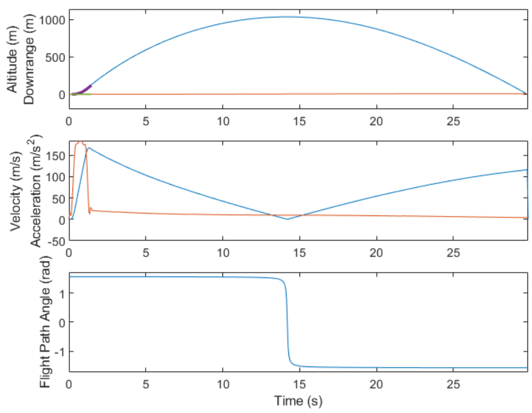

Figure 8: Simulation of the Xi-16 flight on the MATLAB trajectory code.

To validate the trajectory script on a 3-DOF use-case, the same exercise was done, but comparing to the flight profile of SpaceX's Falcon 9 first stage, up until second stage separation, on the SAOCOM-1A mission, flown in 2018. Once more, input uncertainties are not negligible. The aerodynamic coefficients are difficult to estimate for the altitude and speed regimes in which the Falcon 9 flies. Thrust and trajectory data for the launch vehicle was extracted from internet sources that recorded the flight telemetry from the company's live launch webcast.

The outputs from the simulation were compared with the flight data 170 seconds after lift-off, as that was the moment of second stage separation. The results are shown on Table 3.

Table 3: Relative errors between simulated flight and flight telemetry data from the Falcon 9 SAOCOM-1A mission.

Variables at t =170 s	Altitude	Total Velocity	Vertical Velocity
MATLAB tool	94.9 km	2.51 km/s	1.22 km/s
Falcon 9 flight	101 km	1.82 km/s	1.28 km/s
Relative error	6 %	38 %	4.7 %

The tool evidently estimated the horizontal velocity with a substantial error. This could be caused by the aforementioned uncertainties or by a guidance discrepancy, since at the time of this validation exercise, the pitch control script was not yet implemented.

Regarding the multidisciplinary design optimization results, Yamada [3] conducted optimization studies for different objective function weights, for a low altitude sounding rocket. Recent results have confirmed the tool remains useful in that range, after the implementation of the new changes. Optimization studies for other flight envelopes and vehicles sizes are being compiled and preliminary results look favorable.

5. Conclusions

The proposed MATLAB multidisciplinary design optimization framework is a useful tool for the conceptual design (Phase 0, Phase A) of new hybrid propellant rocket vehicles. Given the increasing popularity of hybrid propulsion and new use cases emerging for it, it's predicted this tool will continue to be expanded and developed.

The changes implemented in this work have granted the software a much-needed versatility, allowing it to simulate trajectories in a two-dimensional orbital plane, a requirement for modelling gravity turns of orbital-class booster stages, and establishing the ground works for the introduction of new features, such as throttle control, and reusability.

The trajectory and propulsion disciplines have been updated and validated by comparison with other simulating software and experimental data, with acceptable error rates. On the other disciplines, more work needs to be done in the following weeks and improvements are required to allow the tool to design higher mass and higher apogee vehicles with acceptable errors.

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