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Chemical Reactor Network for Hybrid Rocket Engines Optimization

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This study proposes the integration of a chemical reactor network into the design optimization procedure of hybrid rocket engines. The adoption of a chemical reactor network enables a more realistic representation of combustion phenomena compared to conventional equilibrium-based formulations, by embedding non-ideal effects directly into engine design and performance evaluation. The combustion chamber is discretized into four perfectly stirred reactors (oxidizer-core, fuel-rich, flame and mixer), implemented within the open-source framework Cantera. The network is trained using a particle swarm optimization algorithm against experimental data from the literature on gaseous oxygen and paraffin-based wax propellants, demonstrating high accuracy and predictive capability. The trained chemical reactor network model provides a means to compute the actual characteristic velocity efficiency for each engine configuration considered during optimization, thus improving performance and mass computation during ascent integration. The proposed approach is applied to a reference hybrid rocket upper stage mission, comparing the performance with and without mixing-enhancing devices. Results indicate that a framework based on a chemical reactor network offers a robust foundation for coupled engine–trajectory optimization, enhancing the physical consistency and reliability of hybrid rocket propulsion system design.

Nomenclature

$\mathcal{A}$	=	CRN optimization parameter
A_b	=	burning surface area, m ²
A_{disk}	=	mixing-plate disk area, m ²
A_{holes}	=	total area of the mixing-plate holes, m ²

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A_p	=	port area, m ²
A_{th}	=	nozzle throat area, m ²
a	=	regression constant, m ¹⁺²ⁿ kg ⁻ⁿ s ⁿ⁻¹
$\mathbf{b}$	=	design parameters vector
$\mathbf{b}_L$	=	lower bound vector
$\mathbf{b}_U$	=	upper bound vector
B	=	Spalding transfer number
C_F	=	thrust coefficient
C	=	CRN optimization parameter
c_v	=	specific heat at constant volume, J/(kg K)
$c_{p,gas}$	=	gas specific heat at constant pressure, J/(kg K)
c^*	=	characteristic velocity, m/s
$\mathbf{D}$	=	drag vector, N
D	=	rocket outer diameter, m
D_{post}	=	post-chamber diameter, m
$d_{droplet}$	=	droplet diameter, m
d_{Weber}	=	critical droplet diameter from Weber criterion, m
δ	=	turbulent boundary layer thickness, m
e_j	=	specific internal energy of species j , J/kg
E	=	nozzle expansion area ratio
f	=	PSO fitness function
$\mathbf{F}$	=	thrust vector, N
F	=	mixing fraction of fuel-rich stream entering mixer reactor
F_{min}	=	minimum mixing fraction for purely vapor-phase fuel
$\mathbf{g}$	=	gravity acceleration, m/s ²
G	=	gravitational constant, Nm ² /kg ²
G_O	=	oxidizer mass flux, kg/(m ² s)
$\mathcal{G}$	=	CRN optimization parameter
h	=	altitude, km
h^*	=	target altitude, km
h_{in}	=	specific enthalpy of incoming stream, J/kg
J	=	initial throat area to port area ratio

K_{vap}	=	vaporization constant, m ² /s
K_ϕ	=	mixing-plate loss coefficient
L	=	overall engine length, m
L_b	=	fuel grain length, m
L_{vap}	=	effective heat of vaporization, J/kg
m	=	mass, kg
M	=	Mach number
$M_\oplus$	=	Earth mass, kg
M_j	=	molar mass of species j , kg/kmol
N	=	number
N_{exp}	=	number of experimental test cases
n	=	mass-flux exponent
P	=	burning perimeter, m
p	=	pressure, bar
$\mathcal{P}_{opt}$	=	CRN optimization vector
p_{post}	=	post-chamber pressure, bar
q_c	=	dynamic pressure at grain end, Pa
R	=	specific gas constant of combustion gases, J/(kg K)
$\mathcal{R}$	=	universal gas constant, J/(kmol K)
R_e	=	nozzle exit radius, m
R_g	=	grain outer radius, m
R_i	=	grain initial inner radius, m
R_{th}	=	throat radius, m
$\mathbf{r}$	=	position vector, m
r	=	burning distance, m
T	=	temperature, K
T_{eq}	=	equilibrium gas temperature at mixer inlet, K
$T_{droplet}$	=	droplet surface temperature, K
t	=	time, s
t_{res}	=	gas residence time in combustion chamber, s
t_{vap}	=	droplet vaporization time, s
u_r	=	velocity component in the radial direction, km/s

u_O	= oxidizer velocity in the port, m/s
u_{end}	= gas axial velocity at grain end, m/s
V	= volume, m ³
V_a	= auxiliary helium vessel volume, m ³
V_g	= helium gas volume in oxidizer tank, m ³
v_e	= velocity component in the eastward direction, km/s
$\mathbf{v}$	= velocity vector, m/s
w	= web thickness, m; inertia weight in PSO
$\mathcal{W}$	= inertia weight in PSO
w_n	= velocity component in the northward direction, km/s
Z	= hydraulic resistance, 1/(kg m)
$\mathcal{Z}$	= elemental mass fraction
We	= Weber number
We_{crit}	= critical Weber number for droplet breakup

Greek Symbols

α	= mixture ratio
α_d	= CRN optimization parameter
γ	= specific heat ratio of combustion gases
γ_g	= specific heat ratio of helium
η	= efficiency
η_F	= thrust-coefficient efficiency
λ_{gas}	= gas thermal conductivity, W/(m K)
μ	= payload mass, kg
ρ	= density, kg/m ³
ρ_O	= oxidizer density, kg/m ³
ρ_F	= fuel density, kg/m ³
σ	= surface tension, N/m
Φ	= objective function, kg
ϕ	= latitude, deg

Superscripts

$\cdot$	= time derivative
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Subscripts

0	=	ambient
1	=	combustion chamber at head-end
<i>a</i>	=	auxiliary gas or auxiliary vessel
<i>avg</i>	=	average
<i>bBD</i>	=	before blow-down phase
<i>c</i>	=	combustion chamber
<i>case</i>	=	case
<i>CRN</i>	=	value predicted by the CRN model
<i>dry</i>	=	dry
*	=	characteristic velocity
<i>e</i>	=	nozzle exit
<i>exp</i>	=	experimental value
<i>F</i>	=	fuel
<i>FR</i>	=	fuel-rich reactor
<i>flame</i>	=	flame reactor
<i>g</i>	=	pressurizing gas
<i>gas</i>	=	gas phase property
<i>He</i>	=	helium
<i>i</i>	=	initial value
<i>j</i>	=	j^{th} species
<i>id</i>	=	ideal
<i>max</i>	=	maximum
<i>min</i>	=	minimum
<i>Mixer</i>	=	mixer reactor
<i>nz</i>	=	nozzle
<i>O</i>	=	oxidizer
<i>OR</i>	=	oxidizer-core reactor
<i>p</i>	=	overall propellant (oxidizer + fuel)
<i>post</i>	=	post-chamber
<i>ref</i>	=	reference
<i>res</i>	=	residence-time related quantity
<i>t</i>	=	oxidizer propellant tank

<i>tot</i>	=	total
<i>ull</i>	=	ullage
<i>vap</i>	=	vaporization related quantity
<i>ves</i>	=	vessel
$\oplus$	=	standard astronomical symbol for planet Earth

I. Introduction

HYBRID Rocket Engines (HREs) have emerged as a viable and promising solution in modern propulsion technology, offering performance levels comparable to those of storable and semi-cryogenic liquid rocket systems, with a typical specific impulse of around 300 seconds. By integrating the core advantages of Solid Rocket Motors (SRMs) and Liquid Rocket Engines (LREs), HREs combine cost-effectiveness, operational safety, and throttleability. Moreover, they represent a promising pathway toward more sustainable space transportation in the context of the growing NewSpace economy.

In addition to launch systems, hybrid propulsion is increasingly being considered for in-space applications, such as orbital maneuvering and upper stage propulsion system, thanks to its throttling capabilities and hybrid propellant storability. The ignition of hybrid engines directly in orbit has been validated in recent experimental demonstrations, marking a significant milestone toward their adoption for space missions*. Furthermore, several studies have highlighted the potential of hybrid systems for long-duration and deep-space missions, where operational flexibility and reduced handling constraints are critical[1–3].

Within Europe, environmental regulations are expected to accelerate this green transition. The forthcoming ban on hydrazine and related compounds under the REACH (Registration, Evaluation, Authorization, and Restriction of Chemicals) Regulation is expected to have an estimated €2 billion annual impact on the European space industry†. At the same time, SRMs continue to face scrutiny for their significant environmental footprint, mainly due to the use of chloride-based oxidizers and metallic additives (e.g., aluminum). Hybrid propulsion, by contrast, offers a markedly lower environmental impact. Among the various propellant combinations, liquid oxygen and paraffin-based fuels stand out for their favorable combustion process which emits primarily carbon dioxide, carbon monoxide, and water vapor, leading to lower harmful emissions[4].

Despite these advantages, the widespread adoption of hybrid propulsion has long been limited by technical challenges, particularly low fuel regression rates[5] and combustion instabilities[6, 7]. Recent progress, however, has substantially mitigated these issues: the introduction of liquefying fuels such as paraffin-based wax has enhanced regression rates

*"Hybrid orbital engine ignited in space for the first time in the world", Fergani Space News, 2025. URL: <https://ferganispace.com/en/news/hybrid-orbital-engine-ignited-in-space-for-the-first-time-in-the-world/>, [Online; accessed 30-April-2026]

†"Hydrazine ban could cost Europe's space industry billions, SpaceNews", 2017. URL: <https://spacenews.com/hydrazine-ban-could-cost-europes-space-industry-billions/>, [Online; accessed 3-May-2024]

through the entrainment mechanism[8], while advanced numerical modeling has improved the physical understanding and prediction of combustion instabilities[9].

Global interest in hybrid propulsion is steadily increasing, driven by the goal of closing the performance gap with legacy systems. This trend is reflected in a rapidly expanding body of research[10–12] and in the growing number of dedicated development programs worldwide. In Europe, notable examples include Nammo’s Nucleus sounding rocket, which reached 100 km in 2018, and the NucleusXL launcher under development[13], alongside several EU-funded initiatives under Horizon 2020 and other frameworks, such as ALTAIR, SMILE, HyTEX, HyTEC, HyPrSpace, and ENVOL[‡][14, 15]. Complementary international efforts include Himpulse’s three-stage SL1 launcher[16], whose small-scale demonstrator, named SR75, achieved its first successful suborbital flight in May 2024. Outside the EU, Gilmour Space’s Eris Block 1 (Australia) had its maiden flight in July 2025 (unfortunately unsuccessful) and Reaction Dynamics (Canada) started the testing of the Aurora-8 engines in February 2025[§].

The time and cost associated with hybrid engine development can be substantially reduced through a rigorous conceptual design process. Because propulsion requirements and mission trajectory are closely coupled, hybrid rocket design optimization is inherently multidisciplinary. Furthermore, as single-lever control systems, hybrid engines typically display variable thrust profiles and mixture ratios throughout the burn. Over the past three decades, the Polytechnic University of Torino has built extensive expertise in hybrid propulsion design optimization[17], focusing primarily on multi-stage small satellite launchers and upper-stage applications[18–20], and developing an in-house CFD code [9, 21, 22].

Previous approaches relied on simplified polynomial correlations[18–20] or trained Artificial Neural Networks (ANNs)[23] based on NASA Chemical Equilibrium with Applications (CEA) code outputs to predict engine performance parameters like specific heat ratio, characteristic velocity, and thrust coefficient, assuming chemical equilibrium and frozen flow conditions. In addition, CEA-based approaches have also been used for a preliminary emission estimation of greenhouse gases throughout rocket ascent [4]. While these surrogate approaches improve computational speed compared to direct CEA calls during optimization, they rely on a classical formulation in which the actual characteristic velocity is derived from the ideal one through a constant combustion efficiency, assumed based on literature values [24]. This assumption is not sensitive to engine design and operating conditions and does not account for finite-rate chemistry effects.

This work aims to overcome these limitations by replacing the polynomial-based or ANN-based chemical model with a Chemical Reactor Network (CRN). The CRN approach allows for the incorporation of chemical kinetics and residence time within the combustion chamber, improving the calculation of performance parameters (i.e., the characteristic velocity c^*). The use of a CRN enables this by evaluating residence times according to the actual chamber geometry,

[‡]European Union’s Horizon 2020: ENVOL”, 2022. URL: <https://envol-h2020.eu/>, [Online; accessed 27-May-2022]

[§]Information acquired from: NewSpace Index Website”, 2024. URL: <https://www.newspace.im/launchers/>, [Online; accessed 3-May-2024].

which depends on design variables and varies during engine operation due to regression rate. The proposed model is thus able to account for losses evaluating the completeness of combustion and to capture how factors like mixture ratio, chamber pressure and geometry affect not just the theoretical performance but also the efficiency of energy release.

The proposed CRN-based performance prediction model will be embedded in the optimization procedure for a hybrid-powered upper stage, which is well known and extensively researched by the authors. This test case offers a challenging yet well-understood testbed for assessing the performance of the proposed CRN-based model. The optimization framework will retain the in-house coupled procedure developed at the Polytechnic University of Torino through the years, where an indirect method optimizes the launcher trajectory and an evolutionary approach optimizes the engine design. Two distinct engine architectures will be considered: a baseline configuration without mixing-enhancing devices and an alternative configuration equipped with a mixing plate and a post chamber. This comparison enables the assessment of how combustion completeness and mixing physics, when modeled consistently through the CRN, influence optimal engine sizing and overall mission performance.

The remainder of this paper is organized as follows. Section II introduces the Chemical Reactor Network formulation and the calibration procedure. Section III describes the hybrid-engine performance model, the trajectory optimization framework, and the design variables considered in the coupled problem. Section IV presents the optimization results and discusses the differences between the configurations with and without mixing-enhancing devices. Finally, Section V summarizes the main findings and outlines potential avenues for future research.

II. Chemical Reactor Network Model

Chemical Reactor Networks (CRNs) provide a computationally efficient alternative to full CFD simulations for combustion modeling by discretizing the combustion chamber into interconnected ideal reactors, each representing a distinct physical zone within the chamber. Some applications of CRNs in aerospace propulsion span from pollutant emissions prediction in aero gas turbine engines [25–28] to design optimization tools for supersonic combustors[29]. This work applies the CRN methodology to paraffin-based hybrid rocket combustion. The reactors are built on the physical picture of the flow field established by Marxman et al. in Ref.[30–32] and the mass flow rates between reactors are determined through optimization against experimental data rather than being extracted from CFD data, making the approach particularly valuable when the complete flow fields are unavailable or computationally prohibitive to obtain. This optimization procedure has been explained in detail in Ref.[25] for the simulation of a hydrogen non-premixed burner.

A. Governing Equations

The reactor network is built using the Cantera library [33]. Each reactor in the network is modeled as an adiabatic, constant-volume Perfectly Stirred Reactor (PSR) governed by ordinary differential equations for mass, species, and

energy conservation. The mass conservation equation for each reactor is given by

$$\frac{dm}{dt} = \sum_{in} \dot{m}_{in} - \sum_{out} \dot{m}_{out} \quad (1)$$

where m is the reactor mass and $\dot{m}$ denotes mass flow rates. For each chemical species j , the species conservation equation becomes

$$m \frac{dY_j}{dt} = \sum_{in} \dot{m}_{in} (Y_{j,in} - Y_j) + \dot{m}_{j,gen} \quad (2)$$

where Y_j is the mass fraction of species j and the generation term accounting for chemical reactions is

$$\dot{m}_{j,gen} = V \mathcal{M}_j \dot{\omega}_j \quad (3)$$

with V representing reactor volume, $\mathcal{M}_j$ the molecular weight, and $\dot{\omega}_j$ the net molar production rate computed using detailed finite-rate kinetics from the C1-C3 mechanism for hydrocarbon oxidation developed by the CRECK group [34–36].

The energy conservation equation is

$$m c_v \frac{dT}{dt} = \sum_{in} \dot{m}_{in} \left(h_{in} - \sum_j e_j Y_{j,in} \right) - \frac{pV}{m} \sum_{out} \dot{m}_{out} - \sum_j \dot{m}_{j,gen} e_j \quad (4)$$

where c_v is mixture specific heat at constant volume, p is pressure, h is specific enthalpy, e_j is specific internal energy of species j .

B. Network Topology and Optimization

In our model only the combustion chamber is simulated, neglecting what happens after the nozzle throat. A general scheme of a HRE combustion chamber is provided in Fig. 1: the upper part shows the oxidizer inlet, the pre-chamber, the fuel grain, the port area, the boundary layer, the post chamber and the converging nozzle. The post chamber can generally contain a volume to facilitate mixing, a septum to force mixing, or it could also be absent in lighter configurations. In the lower part, a zoom of the fluid behavior near the fuel grain is provided. The oxidizer core occupies the central region of the port, outside the boundary layer; within the boundary layer, moving from the fuel surface inward, there is a fuel-rich zone, the flame zone, and then an oxidizer-rich zone [37, 38]. In the case of paraffin fuels, on top of the grain there is a melting layer; the hydrodynamic instability at the liquid-gas interface causes entrainment of liquid droplets into the flow, providing an additional mass transfer mechanism beyond surface vaporization and significantly enhancing the regression rate [5].

In our CRN, four distinct reactors capture these essential flow features observed in HREs. Since the CRN uses 0-D

reactors, the flow properties are evaluated at the grain middle section. The fuel-rich reactor represents the boundary layer portion adjacent to the regressing paraffin surface, containing both vaporized fuel and liquid droplets entrained by Kelvin-Helmholtz instabilities at the melt layer interface. The volume of this zone is estimated as 15% of the turbulent boundary layer thickness over the grain length [37]. The flame reactor models the primary combustion zone in the shear layer between fuel-rich and oxidizer streams, with the equivalence ratio maintained to an imposed value through feedback control of the incoming oxidizer flow. This reactor volume is estimated as 10% of the boundary layer volume [37], representing the concentrated reaction zone. The oxidizer-core reactor represents the oxidizer core flow that has not yet mixed with fuel products, with its volume calculated as the remaining port cross-section after subtracting fuel-rich and flame volumes. Finally, the mixer reactor models the post-combustion chamber where final mixing and burnout occur, with the mixing fraction F determining combustion completeness in this zone. The CRN topology is designed to represent these physical zones characteristic of a hybrid rocket combustion and it is represented in Fig. 2.

Four parameters define the mass flow connections between reactors and constitute the optimization vector $\mathcal{P}_{opt} = [\mathcal{A}, C, \mathcal{G}, \alpha_d]$. Parameter $\mathcal{A}$ represents the fraction of total oxidizer flow that diffuses into the fuel-rich boundary layer, parameter C is the fraction of the fuel-rich reactor inlet flow, consisting of diffusion oxidizer and fuel, directed to the primary flame reactor, parameter $\mathcal{G}$ controls the split of residual oxidizer between the mixer and direct bypass to the outlet, and parameter α_d is the droplet atomization factor that scales the liquid particles diameter. The detailed mass flow network begins with the oxidizer stream split into diffusion and bulk components according to

$$\dot{m}_A = \mathcal{A} \cdot \dot{m}_{ox,total} \quad (5)$$

$$\dot{m}_B = (1 - \mathcal{A}) \cdot \dot{m}_{ox,total} \quad (6)$$

where flow $\dot{m}_A$ represents small-scale oxidizer diffusion into the fuel-rich boundary layer and flow $\dot{m}_B$ is the bulk oxidizer entering the core. The fuel-rich reactor feeds the flame according to

$$\dot{m}_C = C \cdot \dot{m}_{fuel} \quad (7)$$

with $\dot{m}_{fuel}$ being the product of the regression rate $\dot{r}$, the burning area A_b and the paraffin density ρ_F . The regression rate is computed using the expression $\dot{r} = a \cdot G_O^n$ developed experimentally by Karabeyoglu in Ref.[39], and at each time step during the simulation the port area and consequently all reactor volumes are updated. The oxidizer flow to the flame is calculated from maintaining the target flame equivalence ratio:

$$\dot{m}_D = \frac{\dot{m}_C \cdot \mathcal{Z}_O^{FR} \cdot (\phi_{fr} - \phi_{flame})}{\phi_{flame}} \quad (8)$$

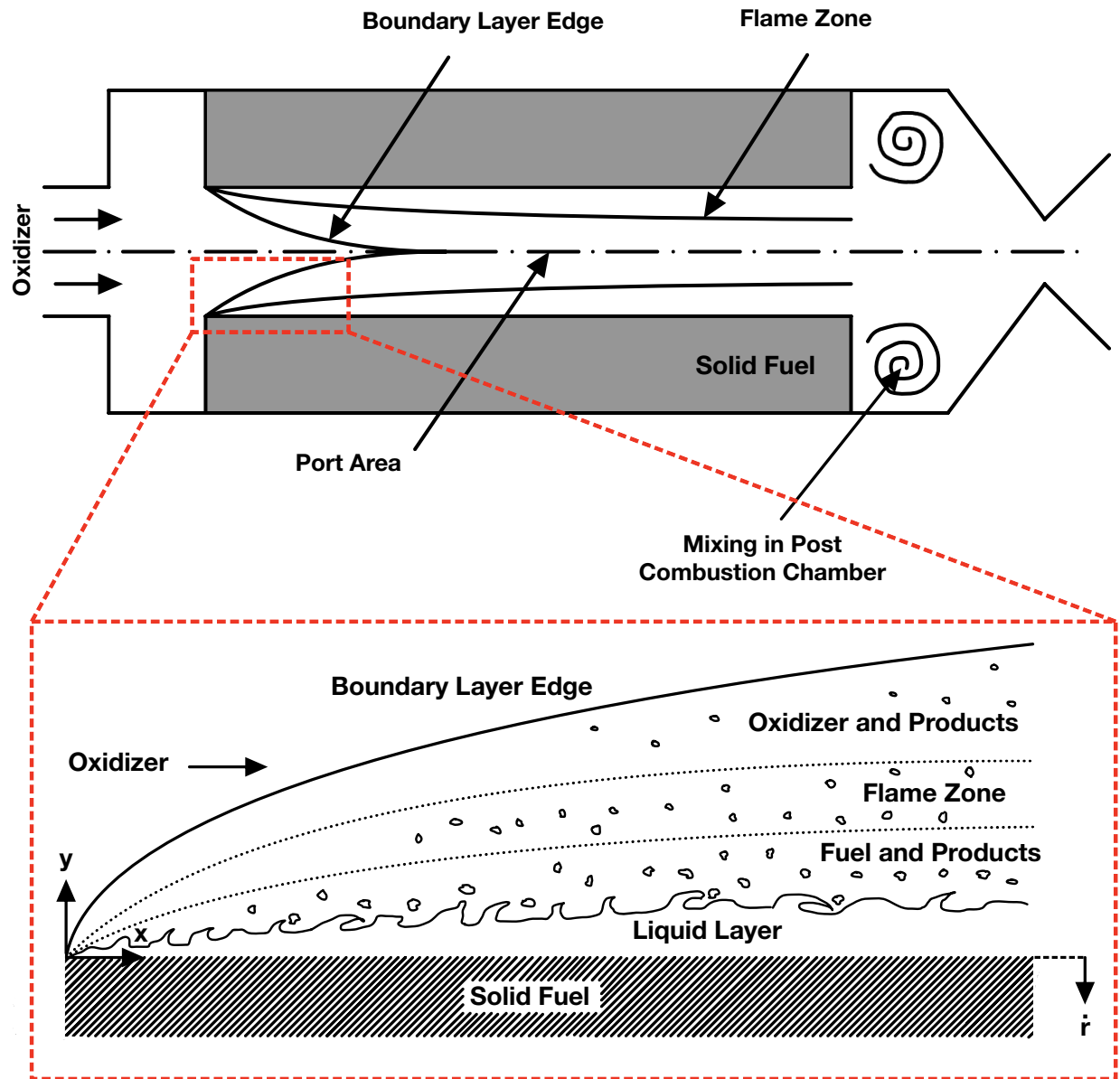


Fig. 1 Schematic of a hybrid rocket engine combustion chamber with liquefying fuel. Adapted from Ref. [37] under CC BY license, <https://creativecommons.org/licenses/by/4.0/>, and from Ref. [38] with permission, Copyright 2007 Joseph Majdalani.

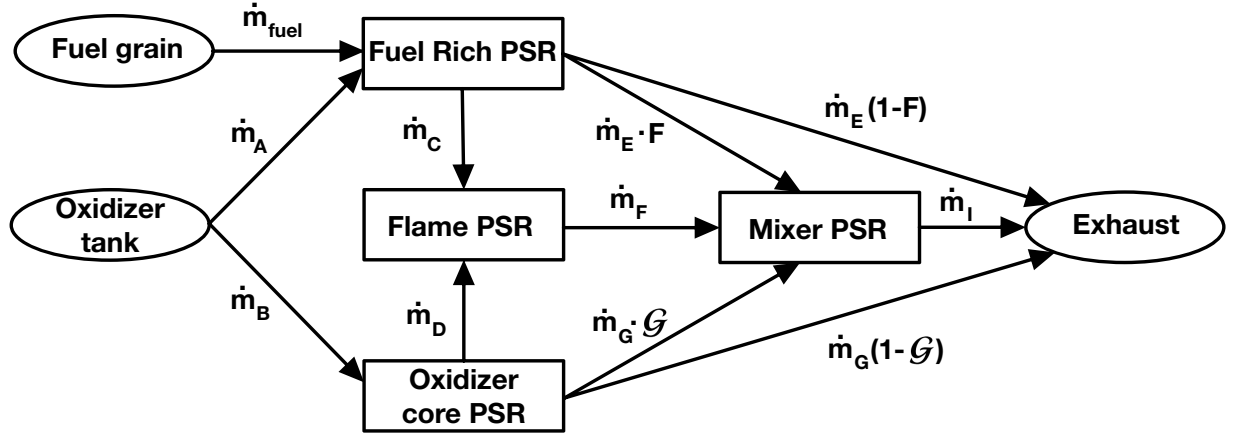


Fig. 2 CRN scheme of the combustion chamber of a HRE.

where ϕ_{fr} is the fuel-rich reactor equivalence ratio, $\phi_{flame} = 2$ is the target flame equivalence ratio, following Ref.[30], and Z_O^{FR} is the oxygen elemental fraction inside the fuel-rich reactor. The fuel-rich outlet stream is $\dot{m}_E = \dot{m}_{fuel} + \dot{m}_A - \dot{m}_C$, which is subsequently split by the fraction parameter F into reacting ($\dot{m}_{E,react} = F \cdot \dot{m}_E$) and non-reacting ($\dot{m}_{E,bypass} = (1 - F) \cdot \dot{m}_E$) components. This captures the fact that part of the fuel does not fully react because a part of paraffin regression rate is due to entrainment of the liquid layer and not all of the droplets are able to vaporize and burn effectively before leaving the combustion chamber. Similarly, the remaining oxidizer after the primary flame, $\dot{m}_G = \dot{m}_B - \dot{m}_D$, is split using parameter G into flows directed to the mixer ($\dot{m}_{G,react} = G \cdot \dot{m}_G$) and directly to the outlet ($\dot{m}_{G,bypass} = (1 - G) \cdot \dot{m}_G$): this models the problem of the oxidizer core not able to properly mix with the fuel in HREs and exiting through the nozzle throat without reacting. The flame products $\dot{m}_F = \dot{m}_C + \dot{m}_D$ combine with the reacting portions of the other streams to give the total mixer inlet flow $\dot{m}_{Mixer,in} = \dot{m}_F + \dot{m}_{E,react} + \dot{m}_{G,react}$.

Optimization is performed using Particle Swarm Optimization (PSO) algorithm [40], which minimizes the error between predicted and experimental characteristic velocity through the fitness function

$$f = \sum_{i=1}^{N_{exp}} \left| \frac{\eta_{CRN,i}^* - \eta_{exp,i}^*}{\eta_{exp,i}^*} \right| \quad (9)$$

where the efficiency $\eta_{CRN,i}^*$ is computed dividing the c^* obtained with the CRN by the ideal c^* obtained at equilibrium conditions with perfect mixing of all reactants. To facilitate CRN modeling and calculation of c_p using NASA polynomials, which are not valid at cryogenic temperatures, oxygen is assumed to enter the combustion chamber in the gaseous phase also when the CRN is embedded in the coupled engine–trajectory optimization. The ideal c^* is calculated using the same initial temperature for reactants to maintain consistency with the CRN model. The c^* inside the CRN is calculated considering the three outlet flows:

$$\Gamma_i = \sqrt{\gamma_i} \left(\frac{2}{\gamma_i + 1} \right)^{\frac{\gamma_i + 1}{2(\gamma_i - 1)}} \quad (10)$$

$$K_{FR} = \frac{\dot{m}_E (1 - F) \sqrt{\frac{T_{FR} \mathcal{R}}{\mathcal{M}_{FR}}}}{\Gamma_{FR}} \quad (11)$$

$$K_{Mixer} = \frac{\dot{m}_I \sqrt{\frac{T_{Mixer} \mathcal{R}}{\mathcal{M}_{Mixer}}}}{\Gamma_{Mixer}} \quad (12)$$

$$K_{OR} = \frac{\dot{m}_G (1 - \mathcal{G}) \sqrt{\frac{T_{OR} \mathcal{R}}{\mathcal{M}_{OR}}}}{\Gamma_{OR}} \quad (13)$$

$$p_{tot} = \frac{K_{FR} + K_{Mixer} + K_{OR}}{A_{th}} \quad (14)$$

$$c^* = \frac{p_{tot} A_{th}}{\dot{m}_E (1 - F) + \dot{m}_I + \dot{m}_G (1 - G)} \quad (15)$$

where $\mathcal{R}$ is the universal gas constant.

The PSO algorithm employs a swarm of 10 particles evolved over 100 generations with cognitive and social acceleration coefficients of $c_1 = c_2 = 2.05$ and inertia weight decreasing linearly from 0.9 to 0.4 [41]. Parameter bounds are set as $0.1 < C < 1$, $0 < \mathcal{G} < 1$, and $0.05 < \alpha_d < 1$. $\mathcal{A}$ was kept fixed to 0.05 to reduce the cost of the optimization procedure.

C. Mixing Fraction Model

The mixing fraction F represents the fraction of fuel-rich stream that effectively burns during the available residence time, capturing vaporization limitations inherent to droplet combustion. Unlike conventional hybrid fuels that rely solely on surface vaporization, paraffin combustion involves entrainment of liquid droplets from the unstable melt layer, and these droplets should vaporize and burn before leaving the combustion chamber to achieve a good combustion efficiency. Thus, vaporization time can be a rate-limiting process in HREs. The idea is to compare the residence time with the time needed for the vaporization to determine how much fuel left in the fuel-rich reactor can actually burn in the mixer reactor.

The residence time in the combustion chamber is calculated as

$$t_{res} = \frac{V_{total} \rho}{\dot{m}_{in}} \quad (16)$$

where V_{total} is the sum of port volume and post-combustion chamber volume, ρ is gas density, and $\dot{m}_{in}$ is the mass flow entering the chamber.

The droplet diameter is estimated from critical Weber number scaling, where the Weber number $We = \rho_{gas} u^2 d / \sigma$ characterizes the relative importance of inertial forces to surface tension forces. Droplets become unstable and break up when $We > We_{crit}$, with bag breakup occurring at $We_{crit} \approx 12$ [42]. The critical diameter corresponding to this threshold is $d_{Weber} = We_{crit} \sigma / (\rho_O u_O^2)$, where ρ_O is oxidizer density and u_O is oxidizer velocity in the port. The actual droplet diameter incorporates enhanced turbulent breakup, extending beyond the standard critical Weber criterion, via:

$$d_{droplet} = \alpha_d d_{Weber} \quad (17)$$

Here, the parameter $\alpha_d < 1$ quantifies the degree of atomization, effectively capturing both the physical enhancement of breakup and the inherent uncertainties in thermodynamic variables and modeling assumptions.

The vaporization time is calculated using [43]:

$$t_{vap} = \frac{d_{droplet}^2}{K_{vap}} \quad (18)$$

where the vaporization constant K_{vap} is

$$K_{vap} = \frac{8\lambda_{gas} \ln(1 + B)}{\rho_F c_{p,gas}} \quad (19)$$

with λ_{gas} representing gas thermal conductivity, ρ_F the fuel density, $c_{p,gas}$ the gas specific heat, and B the Spalding transfer number. The Spalding number is calculated as [43]

$$B = \frac{c_{p,gas}(T_{eq} - T_{droplet})}{L_{vap}} \quad (20)$$

where T_{eq} is the equilibrium temperature calculated from the potential inlet mixture to the mixer reactor before mixing fraction splitting, $T_{droplet}$ is the droplet surface temperature, and L_{vap} is the effective heat of vaporization. The expression used for B assumes negligible thermal inertia of the droplet [44]. Furthermore, for the subset of droplets burning, B should account for the heat of combustion per unit mass of fuel [44]: this effect is included for simplicity in the optimized value for α_d .

The fraction F of the fuel that actually enters the mixer reactor and burns is then calculated as

$$F = F_{\min} + (1 - F_{\min}) \frac{\frac{t_{\text{res}}}{t_{\text{vap}}}}{1 + \frac{t_{\text{res}}}{t_{\text{vap}}}} \quad (21)$$

where parameter $F_{\min} = 0.4$ represents a baseline combustion efficiency including direct vapor-phase fuel that does not undergo droplet entrainment. This value was assumed, as the calibration procedure absorbs any uncertainty in its definition. This formulation ensures correct asymptotic behavior, with $F \rightarrow F_{\min}$ as $t_{\text{res}}/t_{\text{vap}} \rightarrow 0$ and $F \rightarrow 1$ as $t_{\text{res}}/t_{\text{vap}} \rightarrow \infty$, ensuring that a minimum combustion contribution persists even under the most unfavorable residence-time conditions for droplet vaporization.

D. Training and Validation Data

The CRN model is trained against experimental data from the NASA Ames Hybrid Combustion Facility test campaign [39], which demonstrated the high regression rate characteristics of paraffin-based fuels at operationally relevant conditions. The test series employed fuel grains with 7.5 inch (190.5 mm) outside diameter and lengths of 33 or 45 inches (838-1143 mm), operating at chamber pressures from 150 to 1000 psi (10.3-68.9 bar) using gaseous oxygen as the oxidizer, while the fuel formulation SP-1a is a paraffin-based compound with a melting temperature of 342 K.

The regression rate correlation obtained from the tests is $\dot{r} = 0.488 G_O^{0.62}$ (with $\dot{r}$ in mm/s and G_O in g/(cm²·s)).

Five representative test conditions spanning the operational envelope were selected for CRN training: Test 4L-04 operated at $p_c = 45.3$ bar with $\dot{m}_O = 4.44$ kg/s and $L_b = 1.143$ m; Test 4F-3a operated at $p_c = 39.2$ bar with $\dot{m}_O = 4.39$ kg/s and $L_b = 0.838$ m; Test 4L-09 operated at $p_c = 18.3$ bar with $\dot{m}_O = 2.05$ kg/s and $L_b = 1.143$ m; Test 4F-1 operated at $p_c = 36.3$ bar with $\dot{m}_O = 2.03$ kg/s and $L_b = 0.838$ m; Test 4L-12 operated at $p_c = 20.8$ bar with $\dot{m}_O = 2.08$ kg/s and $L_b = 1.143$ m. The other experimental points are used to validate our CRN outside of the conditions in which it was built. These five conditions were selected with the aim of including a diverse set of operating features in the training set, high and low chamber pressure, both grain lengths, and the low- and high-oxidizer-flow regimes, rather than concentrating on a single region of the envelope. The adequacy of this choice is confirmed a posteriori by the leave-one-out cross-validation of Section II.E: removing any single training case and re-fitting leaves the predictive accuracy essentially unchanged, indicating that the calibration does not hinge on any individual test. The largest, though still modest, degradation occurs when test 4F-1 is removed, as it is the only short-grain, low-oxidizer-flow case in the training set and hence the sole anchor for that corner of the operating space.

E. Model Performance and Discussion

The calibrated CRN model demonstrates excellent agreement with experimental data, achieving a mean absolute error of 1% on c^* efficiency across the five training points. The mean error on the validation points is of approximately 1.5%. All the training and validation conditions are summarized in Table 1. The optimization procedure yields parameters $\mathcal{A} = 0.050$, $C = 0.150$, $\mathcal{G} = 0.645$, and $\alpha_d = 0.080$.

Table 1 Comparison of CRN model predictions with experimental data from Ref. [39]. Relative error defined as $\varepsilon = (\eta_{CRN}^* - \eta_{exp}^*)/\eta_{exp}^* \cdot 100$.

Test	P_c [bar]	$\dot{m}_O$ [kg/s]	O/F	$D_{port,mean}$ [m]	L_{grain} [m]	D_{throat} [m]	η_{exp}^*	η_{CRN}^*	ε [%]	Dataset
4F-1	36.3	2.03	3.05	0.1345	0.838	0.0371	0.85	0.864	+1.65	Training
4F-1a	34.5	4.02	3.89	0.1551	0.838	0.0503	0.91	0.892	-1.98	Validation
4F-1b	38.7	2.13	2.72	0.1373	0.838	0.0368	0.85	0.845	-0.59	Validation
4F-1c	37.4	2.07	3.00	0.1526	0.838	0.0368	0.89	0.845	-5.06	Validation
4F-4	36.3	4.24	3.97	0.1345	0.838	0.0503	0.90	0.899	-0.11	Validation
4F-5	38.0	4.32	3.54	0.1297	0.838	0.0503	0.88	0.880	+0.00	Validation
4F-3a	39.2	4.39	3.84	0.1458	0.838	0.0503	0.90	0.889	-1.22	Training
4L-01	46.3	4.40	2.57	0.1440	1.143	0.0503	0.88	0.846	-3.86	Validation
4L-03	44.3	4.45	2.69	0.1603	1.143	0.0503	0.84	0.849	+1.07	Validation
4L-04	45.3	4.44	2.66	0.1239	1.143	0.0503	0.85	0.854	+0.47	Training
4L-05	44.7	4.43	2.72	0.1318	1.143	0.0503	0.85	0.856	+0.71	Validation
4L-08	36.2	4.42	2.64	0.1341	1.143	0.0562	0.85	0.854	+0.47	Validation
4L-09	18.3	2.05	1.70	0.1166	1.143	0.0556	0.80	0.791	-1.13	Training
4L-10	40.7	5.55	2.89	0.1480	1.143	0.0613	0.88	0.863	-1.93	Validation
4L-12	20.8	2.08	2.01	0.1173	1.143	0.0513	0.79	0.794	+0.51	Training

The robustness of the five-point calibration was assessed by leave-one-out cross-validation. In each of the five folds one training test is removed, the PSO is re-run on the remaining four conditions, and the calibrated model is scored through three c^* -efficiency error metrics: the train MAPE, the mean absolute percentage error in η_{CRN}^* over the four retained tests; the LOO error, the absolute relative error on the single withheld test; and the validation MAPE, the mean absolute percentage error over the independent ten-test hold-out set, which enters no calibration. Table 2 reports the recovered parameters and the three metrics for every fold, with the nominal five-point calibration as baseline; the daggered entries reached the lower optimization bounds ($C \geq 0.10$, $\alpha_d \geq 0.05$).

Every reduced four-point fit reproduces its own training tests to better than 1% (Train MAPE = 0.42–0.91%), and the hold-out accuracy is essentially fold-independent: the Val MAPE stays between 1.43% and 2.16%, a total spread of 0.7 % within which the baseline value of 1.57% falls. No single training condition is therefore decisive for generalization. The parameter $\mathcal{G}$ is recovered consistently across folds (0.625–0.660), identifying it as the dominant, well-constrained

Table 2 Leave-one-out cross-validation of the five-point CRN calibration.

Left-out	C	$\mathcal{G}$	α_d	Train MAPE [%]	LOO error [%]	Validation MAPE [%]
4L-12	0.181	0.641	0.121	0.59	1.45	2.07
4F-3a	0.210	0.625	0.112	0.42	2.13	2.16
4L-09	0.180	0.631	0.105	0.68	1.15	2.08
4F-1	0.100 [†]	0.660	0.050 [†]	0.73	2.98	1.43
4L-04	0.193	0.634	0.119	0.91	0.28	2.14
Baseline	0.150	0.645	0.080	1.00	—	1.57

degree of freedom. By contrast C and α_d cluster tightly in four folds ($C = 0.180\text{--}0.210$, $\alpha_d = 0.105\text{--}0.121$) but fall to their lower bounds ($C = 0.100$, $\alpha_d = 0.050$) in the single fold where 4F-1 ($p_c = 36.3$ bar, $\dot{m}_O = 2.03$ kg/s) is withheld. The 4F-1 test is also the least reproducible point: its LOO error of 2.98% is the largest of all folds and 1.3 % above the error it shows when retained in training, identifying it as the condition that anchors C and α_d away from their lower bounds in the region of moderate chamber pressure and low oxidizer mass flow. Tellingly, that same fold returns the lowest hold-out error (1.43%) even with C and α_d at their bounds: over this range η_{CRN}^* is only weakly sensitive to C and α_d individually and is governed chiefly by $\mathcal{G}$. With burn-averaged data the calibration thus resolves one strongly identified parameter ($\mathcal{G}$) and a pair (C , α_d) that is well constrained only when 4F-1 is present.

The CRN is integrated in time: the simulation is initialized at the mean port radius of each test, computed as the arithmetic average of the initial and final radii using the experimentally reported regression rate and burn time. Starting from this geometry, Cantera advances the reactor ODEs with a time step $\Delta t = 5 \times 10^{-5}$ s; at every ODE time step the port area and all reactor volumes are updated through $\dot{r} = a G_O^n$, so the model intrinsically resolves the time-dependent efficiency $\eta^*(t)$ over the 0.1 s integration window. The burn-averaged CRN characteristic velocity is the time-mean of $c^*(t)$ over that window; the efficiency η_{CRN}^* , shown in Table 1, is then obtained by dividing this value by the ideal c^* computed separately via chemical equilibrium at the experimentally reported mean mixture ratio and mean chamber pressure of each test. This approach is similar to the one reported in Ref. [39], where η_{exp}^* is defined as the ratio of the burn-averaged measured c^* to the ideal c^* at mean operating conditions, so model and experiment are compared on a consistent footing.

The averaging window is set to 0.1 s to reduce computational cost: a single evaluation then costs $\approx 2 \times 10^{-3}$ CPU-hours, keeping the several thousand network evaluations required by the PSO calibration computationally tractable. To confirm that this window is appropriate, each test was additionally simulated with longer integration windows of 1.0 and 2.0 s. Because the parameters are fitted at the 0.1 s window, agreement there is built in, so these longer runs serve as a consistency check rather than an independent validation; across them η_{CRN}^* shifts by little more than 1 %. The grain regresses during these integrations, the port opening through the regression law $\dot{r} = a G_O^n$, so the check genuinely

exercises the time-dependence the model already contains, and the small drift shows that this geometric evolution moves η_{CRN}^* gradually rather than abruptly. The effects that would make a longer window genuinely worthwhile are the ones presently omitted: chiefly nozzle-throat erosion, a cumulative process whose influence on chamber pressure, and hence on η_{CRN}^* , builds up only over the full burn; and, more subtly, the slow evolution of turbulent mixing, since the partially stirred reactor here sets conversion from the residence and droplet-vaporization times and could be extended with a mixing-length estimate of the turbulent mixing time. With these effects absent, the 0.1 s window faithfully represents the modeled physics at a small fraction of the cost; incorporating throat erosion in particular would supply a physically sound reason to integrate over the whole burn, and is left to future work.

Current results are based on five training points covering a limited range of operating conditions. The model assumes the network topology remains valid across operating conditions. Additional validation across a wider range of chamber pressures, grain lengths, and oxidizer-to-fuel ratios is recommended to fully establish the model's predictive capability and generalizability to diverse hybrid rocket configurations.

III. Numerical Model for Trajectory Optimization

A. Engine

A hybrid rocket engine suitable as an upper stage for the Vega launcher is considered as a reference case. The initial mass of the stage is given ($m_i = 14522$ kg)[¶] The propellants are Liquid O₂gen (LOX) and paraffin-based wax (C₃₂H₆₆). This propellant combination is very promising for HREs due to its specific impulse in the 300-second range and high regression rate [5], thus avoiding complex multi-port grain designs and the use of aluminum particles that would compromise the eco-friendliness of the exhaust gases. In order to maintain a simple system design, a partially regulated feeding is used for the liquid oxygen: initially, the hybrid engine works at a constant tank pressure thanks to a pressurant flow from an auxiliary vessel, followed by a relatively short Blow-Down (BD) phase.

The engine modeling is based on a set of proper assumptions and hypotheses:

- 1) $\eta_F = 0.98$, accounting for losses in the evaluation of the thrust coefficient C_F [24];
- 2) frozen equilibrium expansion in the nozzle, i.e., $\gamma = \text{constant}$;
- 3) isentropic expansion in the nozzle [24];
- 4) single circular port grain design, uniform regression rate along port axis, and no contribution of grain lateral ends to overall combustion;
- 5) regression rate correlation coefficient $a = 9.1 \cdot 10^{-5} \text{ m}^{2n+1} \text{ s}^{n-1} \text{ kg}^{-n}$ and exponent $n = 0.69$ [5] (SI units);
- 6) third-order polynomial fittings of $c_{id}^*(\alpha)$, $\gamma(\alpha)$, $R(\alpha)$, and $T_c(\alpha)$ (computed by NASA CEA with $p_c = 10$ bar = constant) [45];

[¶]Data are acquired from: Arianespace, "VEGA, User's Manual, Issue 4 - Revision 0", 2014. URL: http://www.arianespace.com/wp-content/uploads/2015/09/Vega-Users-Manual_Issue-04_April-2014.pdf, [Online; accessed 2-July-2019].

- 7) hydraulic resistance $Z = \text{constant}$ and incompressible turbulent flow in the tank-chamber flow path;
- 8) $(p_c)_i = 0.4(p_t)_i$ to avoid the coupling between the engine and the feed system during operation;
- 9) $J = A_{th}/A_p = 0.5$ at engines ignition to limit pressure losses in the combustion chamber;
- 10) no erosion of nozzle throat and mixing plate orifices (when employed);
- 11) initial ullage volume V_{ull} equal to 3% of the overall oxidizer volume[46];
- 12) initial auxiliary helium vessel pressure $(p_a)_i = 250 \text{ bar}$;
- 13) oxidizer tank pressure $p_t = 25 \text{ bar} = \text{constant}$ during the regulated operation;

The c-star efficiency η^* is given by the CRN (see the Sec.II) for the mixerless engine design, whereas $\eta^* = 0.96$ has been assumed when mixing devices are taken into account (see the Subsec.III.B).

Six input design parameters give the engine design under these assumptions: grain outer radius R_g , web thickness w , grain length L_b , the overall oxidizer mass exhausted $(m_O)_f$, the oxidizer mass exhausted during the BD operation $(m_O)_{bBD}$, and the nozzle expansion area ratio E . The input parameters are collected in:

$$\mathbf{b} = [R_g, w, L_b, (m_O)_f, (m_O)_{bBD}, E] \quad (22)$$

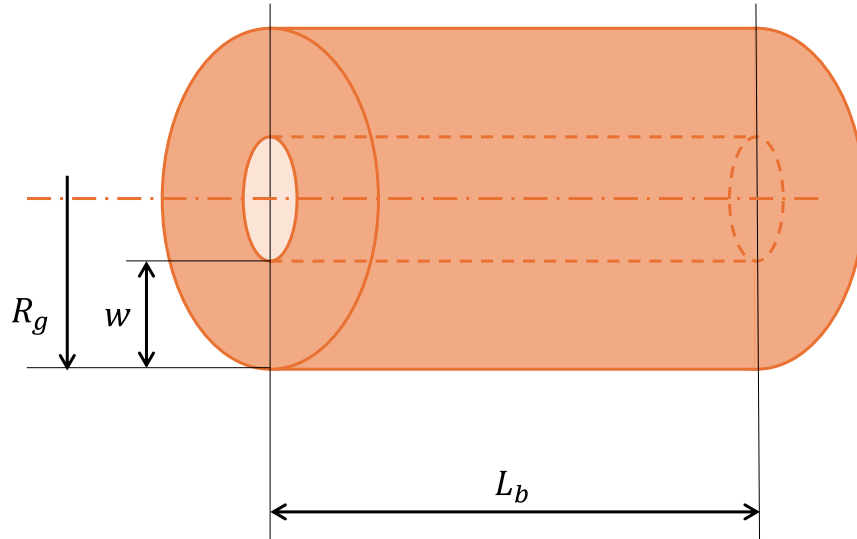


Fig. 3 Fuel grain geometry and design parameters.

The fuel grain geometry is determined by R_g , w , and L_b as depicted in Fig. 3. The grain inner radius is then $R_i = R_g - w$. The burning perimeter P and the port area A_p can be evaluated for any given burning distance r ($0 \leq r \leq w$) as:

$$P = 2\pi (R_i + r) \quad (23)$$

$$A_p = \pi (R_i + r)^2 \quad (24)$$

An approximate relation accounts for pressure losses inside the combustion chamber [47]:

$$p_1 = \left[1 + 0.2 \left(\frac{A_{th}}{A_p} \right)^2 \right] p_c \quad (25)$$

where p_c is the chamber nozzle-stagnation pressure, p_1 is the chamber head-end pressure, and A_{th} is the nozzle throat area. Oxidizer mass flow rate $\dot{m}_O$ is given by:

$$\dot{m}_O = \sqrt{(p_t - p_1)/Z} \quad (26)$$

where p_t is the oxidizer tank pressure. The hydraulic resistance Z (assumed constant) is evaluated to satisfy the initial decoupling condition between the combustion chamber and the feed line. Grain geometry and $\dot{m}_O$ determine the fuel regression rate $\dot{r}$:

$$\dot{r} = a (\dot{m}_O/A_p)^n \quad (27)$$

Fuel mass flow rate $\dot{m}_F$ is then:

$$\dot{m}_F = \rho_F \dot{r} A_b = \rho_F \dot{r} L_b P \quad (28)$$

where ρ_F is the fuel grain density (940 kg/m³ for paraffin-based wax), and A_b is the burning area. The instantaneous mixture ratio α is:

$$\alpha = \frac{\dot{m}_O}{\dot{m}_F} \quad (29)$$

whereas the time-averaged mixture ratio $\bar{\alpha}$ as function of the design parameters is:

$$\bar{\alpha} = \frac{(m_O)_f}{\pi(R_g^2 - R_i^2)L_b\rho_F} = \frac{(m_O)_f}{\pi(2R_g w + w^2)L_b\rho_F} \quad (30)$$

Characteristic velocity $c^*(\alpha) = \eta^* c_{id}^*(\alpha)$ is known, and thus chamber pressure p_c :

$$p_c = \frac{(\dot{m}_O + \dot{m}_F)c^*}{A_{th}} \quad (31)$$

The oxidizer tank is pressurized by helium supplied from an auxiliary vessel with volume V_a and initial pressure p_a . Although V_a is a design parameter, it is conveniently expressed in terms of the oxidizer mass that has been exhausted at the start of the BD phase, $(m_O)_{bBD}$. A regulation valve maintains $p_t = (p_t)_i$ throughout the regulated operating phase. During the following BD phase, p_t is computed assuming an isentropic expansion of the helium within the oxidizer tank:

$$p_t = (p_t)_i \left[\frac{(V_g)_{bBD}}{V_g} \right]^{\gamma_g} \quad (32)$$

Here, the generic helium volume in the tank at time t is given by $V_g(t) = (V_g)_i + m_O(t)/\rho_O$, which depends on the oxidizer mass $m_O(t)$ exhausted up to that time. At the beginning of the BD phase, $(V_g)_{bBD} = (V_g)_i + (m_O)_{bBD} / \rho_O$, and γ_g denotes the specific heat ratio of helium.

The thrust coefficient C_F is calculated as:

$$C_F = \eta_F \left\{ \sqrt{\frac{2\gamma^2}{\gamma-1} \left(\frac{2}{\gamma+1} \right)^{\frac{\gamma+1}{\gamma-1}} \left[1 - \left(\frac{p_e}{p_c} \right)^{\frac{\gamma-1}{\gamma}} \right]} + E \frac{p_e}{p_c} \right\} - E \frac{p_0}{p_c} \quad (33)$$

It is worth noting that the term related to the atmospheric pressure, i.e., p_0/p_c , is always small since the upper stage always flies at high altitude. Propellant mass flow rate at ignition (i.e., at $t=0$) $(\dot{m}_p)_i$ can be found as:

$$(\dot{m}_p)_i = (1 + \alpha_i)(\dot{m}_F)_i = \frac{1 + \alpha_i}{\alpha_i} (\dot{m}_O)_i \quad (34)$$

Nozzle throat area A_{th} and initial port area $(A_p)_i$ are given by:

$$A_{th} = \frac{(\dot{m}_p)_i}{(p_c)_i c_i^*} ; \quad (A_p)_i = \frac{A_{th}}{J} \quad (35)$$

For the interested reader, a schematic of the engine model is shown in Fig. 4.

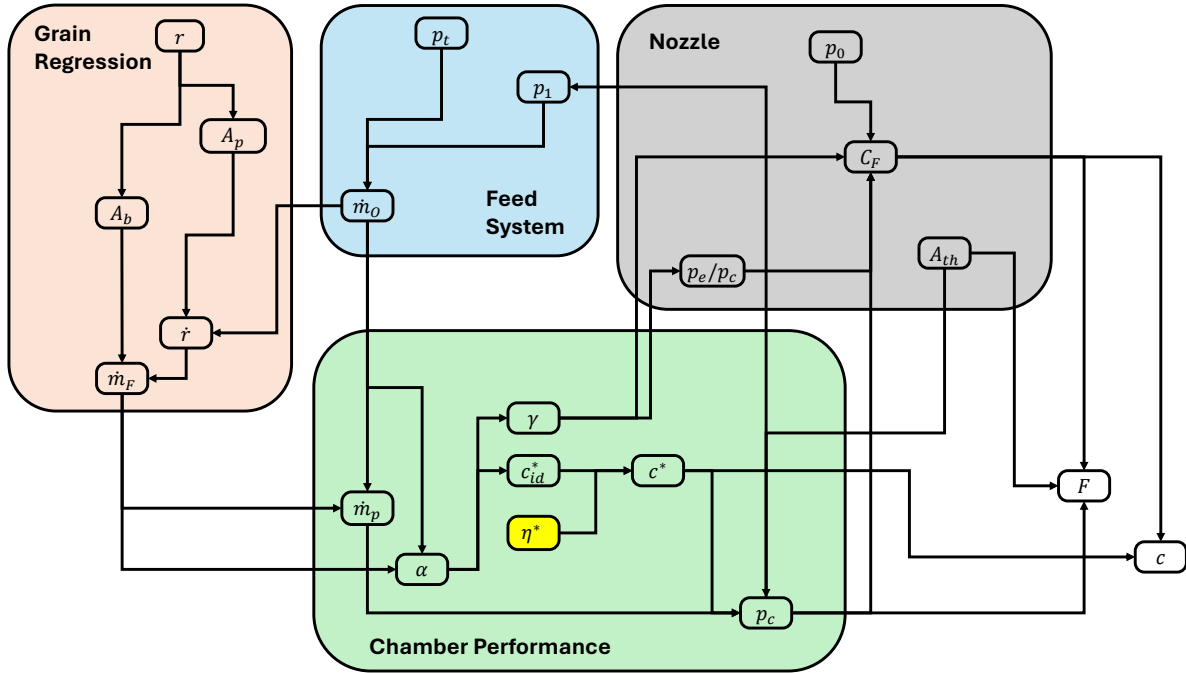


Fig. 4 Visual representation of the engine model during operation.

It is now useful to introduce the upper and lower boundary vector for the design variables $\mathbf{b}_U$ and $\mathbf{b}_L$, shown

in Table 3. The bounds of the design variables define the explored design space and have been selected based on a combination of application-driven constraints and prior experience with evolutionary optimization techniques on the same test case. In particular, some limits are imposed by strict geometrical and integration requirements and are therefore not relaxed during the optimization (e.g., the maximum value of $2R_g$ is constrained by the upper-stage diameter of the reference launcher). Other bounds, instead, are introduced to improve the convergence of the evolutionary algorithm by restricting the exploration of non-viable regions. For these parameters, the initial ranges were intentionally selected to be relatively narrow and were iteratively expanded during the early optimization runs whenever candidate optimal solutions consistently approached or reached the imposed limits, ensuring that the final solutions were not artificially constrained by the initial choice of these bounds.

Table 3 Design parameters ranges.

	R_g [m]	w [m]	L_b [m]	$(m_O)_f$ [kg]	$(m_O)_{bBD}$ [kg]	E
b_L	0.57	0.25	4.00	6100	3195	15
b_U	0.60	0.32	4.50	7697	5083	20

B. Mixer

HREs typically suffer from incomplete combustion due to their diffusion-limited combustion process, which restricts the proper mixing of oxidizer and fuel. This limitation is commonly accounted for in the characteristic velocity c^* by introducing the so-called c-star efficiency η^* . In classical rocket propulsion theory, η^* is used to quantify departures from ideal combustion performance and is often assumed to be close to unity in preliminary analytical models (e.g., 0.96 in Ref. [24]). This convention is adopted by several HRE performance numerical studies in the most modern literature [48–50].

In practice, however, η^* rarely exceeds 0.85-0.90 in experimental tests without dedicated flow-enhancing devices. Conversely, the use of diaphragms or other mixing devices along the fuel grain or in the post-combustion chamber can promote turbulent recirculation, extend residence times and enhance species mixing, thus increasing η^* . Bellomo et al. [51] demonstrated that a diaphragm positioned in the first third of the fuel grain length generates recirculation zones strong enough to increase local reaction rates, produce thicker flames, and enhance fuel regression. Their simulations exhibited a measurable performance gain due to the diaphragm, with η_* improved by up to 5% relative to the baseline configuration without any flow-enhancing devices.

In Ref. [52], the effects of diaphragm position and diameter were investigated. The results showed that reducing the orifice diameter (from 50 mm to 20 mm) nearly doubled the local regression rate and raised η^* from below 90% to almost unity (98.9%). These results suggested a quadratic relationship between η^* and the blockage ratio of the diaphragm opening, with diminishing returns as the device is positioned closer to the nozzle.

Zilliac et al. [53] analyzed a comprehensive set of literature data and dedicated Peregrine hot-fire tests to demonstrate that the dominant factor controlling η^* is the degree of turbulent mixing within the combustion chamber. Configurations incorporating geometrical mixing elements (such as steps, screens, diaphragms, or post-chamber mixers) systematically exhibited higher efficiencies than those without, with an average increase of about 11% in the surveyed dataset. The Peregrine campaign itself demonstrated a burn-averaged efficiency close to 95% for a configuration equipped with an efficiency-enhancing device. These results underline that properly placed mixing devices can raise combustion completeness toward values commonly assumed in performance models. However, mixing devices frequently introduce additional axial pressure losses (typically in the range 5–10%), locally enhance regression downstream of the device (if placed along the grain), and can modify surface and thermal conditions affecting nozzle erosion and long-duration survivability. For these reasons, post-grain mixing devices are generally preferable, as they have fewer adverse effects on regression rate and heat transfer. Nevertheless, the added mass and pressure loss introduced by such devices should be carefully considered in system-level sizing and optimization alongside the anticipated improvements in η^* . To explore these engineering trade-offs, two hybrid engine architectures are examined in this work.

The first is a mixerless configuration, in which no mixing-enhancing device or dedicated post chamber is included in the design. Rocket performance is evaluated following Sec. III.A, where η^* is estimated using the aforementioned CRN approach as a function of the average combustion chamber geometry (defined by the average port diameter, nozzle throat diameter, and grain length) and the operating conditions (time-averaged mixture ratio). In this way, each tentative engine design corresponding to a given vector $\mathbf{b}$ is assigned a specific (though constant) value of η^* .

The second architecture includes mixing-enhancing devices. In this configuration, the hybrid rocket incorporates a four-hole diaphragm located at the end of the grain, followed by a post-chamber designed to achieve high values of η^* . The design and mass estimation of these components rely on the following assumptions. The post-chamber diameter D_{post} is set equal to the combustion chamber diameter, while its length is taken as 30% of that diameter. Both the mixing plate and the post-chamber walls are assumed to be made of Inconel 718. Carbon-phenolic ablative layers are applied to the post-chamber walls, inside the mixing-plate holes, and on the front and rear faces of the disk. The post-chamber wall thickness is sized to withstand the internal post-chamber pressure p_{post} , which is assumed to be 90% of the initial chamber pressure at ignition. Literature indicates that such a 10% pressure drop across the plate is sufficient to achieve nearly complete mixing, corresponding to η^* close to unity. Following Ref. [24], a target value of $\eta^* = 0.96$ is imposed, and the diaphragm design is determined accordingly.

The CRN calibration in Sec. II is based on the Stanford/NASA Ames GOX/paraffin data set, which does not include mixing-enhancing devices. Therefore, the CRN-predicted c^* -efficiency is used only for the mixerless configuration. The mixer-equipped architecture is modeled separately by prescribing $\eta^* = 0.96$, consistently with literature values for diaphragm/passive-mixer configurations, while accounting for the associated pressure loss and hardware mass, as described in the following.

The pressure drop due to the mixing plate at ignition can be expressed as

$$\left[\frac{\Delta p}{(p_c)_i} \right]_{required} = K_\phi (q_c)_i, \quad (36)$$

where $(q_c)_i = \frac{1}{2} \gamma (p_c)_i M_{end}^2$ is the dynamic pressure of the combustion products at the grain exit, and $K_\phi = \left(\frac{1}{\phi^2} - 1 \right)^{0.5}$ is a classical short-hole loss correlation [54]. The Mach number at the grain end is $M_{end} = u_{end}/c_{end}$, where u_{end} is computed from $(\dot{m}_p)_i$, $(A_p)_i$, and $(\rho_c)_i$, and the sound velocity at grain end c_{end} is obtained from γ , R , and T_c using polynomial fits of NASA CEA results.

The corresponding hole diameter is

$$d_{holes} = D_{post} \left(\frac{\phi}{n_{holes}} \right)^{0.5}, \quad (37)$$

where $\phi = A_{holes}/A_{disk}$ is the hole-to-disk area ratio. During operation, the pressure drop is updated assuming a constant value of K_ϕ (erosion effects are neglected) and is evaluated using the instantaneous chamber pressure p_c .

The presence of the mixing plate must also be included in the thrust coefficient evaluation:

$$C_F = \frac{F}{p_c A_{th}} = \frac{F}{p_{post} A_{th}} \frac{p_{post}}{p_c} = C_F^* \left(\gamma, E, \frac{p_e}{p_{post}}, \frac{p_0}{p_{post}} \right) \left(1 - \frac{\Delta p}{p_c} \right), \quad (38)$$

where C_F^* is the thrust coefficient computed as in Eq. 33, but using the upstream pressure p_{post} (i.e., the pressure downstream of the mixing plate) instead of the chamber pressure p_c .

C. Mass Budget, Trajectory and Optimization

The initial mass of the upper stage m_i is specified at the ignition of the hybrid upper stage. The stage dry mass m_{dry} and propellant mass m_p are given by the design parameters $\mathbf{b}$, and the payload mass is then $\mu = m_i - m_{dry} - m_p$. The masses of the engine components are estimated through appropriate assumptions and approximations. The combustion chamber includes a 6-mm insulating liner with the same density as the solid fuel and an aluminum alloy cylindrical wall. The oxidizer tank is an aluminum cylinder with a 1.9-m diameter, equal to that of Vega's third stage, and the pressurizing gas is stored in a spherical aluminum tank. The wall thicknesses of the tanks and chamber are designed to withstand internal operating pressure with a safety factor of 1.25. Additionally, the HRE is enclosed in a 1-mm-thick cylindrical aluminum casing, and a nozzle with a 45° convergent and 20° divergent section coated with an ablative layer is adopted. A uniform thickness is assumed and computed following Ref. [55], using average transport properties and the estimated heat flux at ignition. These conservative assumptions lead to an overestimation of the nozzle mass. The structural mass of the nozzle is small compared to the ablative layer and is therefore neglected. In the end, the mass of the post chamber and mixing plate are calculated as depicted in the subsec. III.B, when employed in the engine design.

An in-house indirect method based on the optimal control theory optimizes the trajectory, aiming at the maximization

of the insertion altitude h for the given engine performance and mass budgeting. A point mass rocket is considered and the derivative of position $\mathbf{r}$ (radius, latitude, and longitude), velocity $\mathbf{v}$ (radial, eastward, and northward components), and rocket mass m [56] are given by the following vectorial state equations:

$$\frac{d\mathbf{r}}{dt} = \mathbf{v} \quad \frac{d\mathbf{v}}{dt} = \mathbf{g} + \frac{\mathbf{F} - \mathbf{D}}{m} \quad \frac{dm}{dt} = -\frac{|\mathbf{F}|}{c^* C_F} \quad (39)$$

An inverse-square gravity field is assumed:

$$\mathbf{g} = -\frac{GM_{\oplus}}{||\mathbf{r}||^3} \mathbf{r} \quad (40)$$

where G is the gravitational constant and $M_{\oplus}$ is Earth mass.

Density and pressure are obtained by interpolating standard atmosphere tables as functions of rocket altitude during ascent. The equations of motion are expressed in non-dimensional form to enhance numerical integration accuracy. Details of the indirect optimization procedure are provided in Ref. [57].

The conditions at the ignition of the hybrid upper stage, consistent with a launch from Kourou, are assigned: altitude $h = 86.88$ km, latitude $\phi = 9.11^\circ$, velocity components in the radial, eastward and northward directions $u_r = 0.142$ km/s, $v_e = 0.230$ km/s, $w_n = 4.146$ km/s, respectively. Eccentricity and inclination of the target orbit are imposed (zero and 90 deg. respectively), whereas the longitude of the ascending node is left free.

The reference mission here considered has an expected target orbit of 700 km, in analogy to Vega Launcher's specifications. Thus, once the hybrid upper stage performance are known (i.e., the payload mass μ and the insertion altitude h), a performance index Φ can be computed as:

$$\Phi = \mu - k \cdot \max(0, \Delta_h) \quad \text{where } \Delta_h = h^* - h \quad (41)$$

where an ϵ -constraint approach is used to maximize μ and force altitude violation Δ_h to zero ($k = 20$ kg/km, $h^* = 700$ km).

The hybrid engine design optimization is performed using a Particle Swarm Optimization (PSO) algorithm developed in Fortran within the Aerospace Propulsion Group at the Polytechnic University of Torino and refined over the years [58, 59]. The PSO algorithm is a stochastic optimization technique inspired by the collective behavior of biological populations such as flocks of birds or schools of fish [60, 61]. Each particle represents a potential solution within the design space and adjusts its trajectory based on information gathered from both its own experience and that of the entire swarm. This information-sharing mechanism enhances convergence capabilities compared with other classes of population-based algorithms, such as genetic algorithms.

The proposed implementation incorporates Trelea's improvements to PSO [41], aiming for an optimal balance between exploration and exploitation of the design space. A high initial inertia weight, $w_{max} = 0.95$, promotes broad

exploration, while a lower final inertia weight, $w_{min} = 0.4$, enables fine exploitation of the most promising regions once good solutions have been identified. During the optimization process, the inertia weight at the i -th iteration, w^i , is updated as a function of the maximum number of iterations, N_{max} , according to:

$$w^i = w_{max} - (i/N_{max})(w_{max} - w_{min}) \quad (42)$$

Along with the inertia weight, the PSO algorithm employs two acceleration coefficients, namely the cognitive acceleration c_1 and the social acceleration c_2 , to update each particle's velocity and position. The cognitive component c_1 represents a particle's self-confidence, attracting the k -th particle toward its own best-known position, $p_{k,best}$. The social component c_2 represents the attraction toward the global best position, g_{best} , discovered by the entire swarm. In this work, the authors adopt $c_1 = c_2 = 2$.

The velocity of the k -th particle, v_k , is updated during the optimization process as:

$$v_{k+1} = w^i \cdot v_k + c_1 \cdot r_1 \cdot (p_{k,best} - p_k) + c_2 \cdot r_2 \cdot (g_{best} - p_k) \quad (43)$$

where p_k is the position of the k -th particle and w^i is the inertia weight at the i -th iteration. r_1 and r_2 are uniformly distributed random numbers in the range $[0, 1]$, which introduce stochasticity into the algorithm at each iteration.

Before updating the particle positions, the velocities are clipped to $v_{max} = 0.25 (\mathbf{b}_U - \mathbf{b}_L)$, where $\mathbf{b}_U$ and $\mathbf{b}_L$ are the upper and lower bounds of the design variables, respectively. Introducing v_{max} helps maintain an appropriate balance between exploration (broad search of the design space) and exploitation (local refinement around promising solutions). Twenty particles and 1000 generations are used in this work, corresponding to approximately 50 CPU hours per optimization run (CPU: Intel(R) i7-9700 @ 4 GHz). Multiple runs were carried out to increase confidence in convergence toward a global optimum.

IV. Results

The hybrid engine design parameters for the optimal solutions obtained from the optimization process are reported in Table 4. The corresponding mass budget, key parameters, and performance metrics are summarized in Table 5 and Table 6. In addition, Figs. 5–7 present the main engine operating parameters as functions of time, namely thrust F , propellant mass flow rate $\dot{m}_p$, specific impulse I_{SP} , mixture ratio α , characteristic velocity c^* , and thrust coefficient C_F .

To achieve insertion into the target orbit, the hybrid engine performs two distinct burns. However, the second burn is very short (about 10 s) compared to the first one and has a negligible impact on overall propellant consumption and engine design tradeoffs. For this reason, all Figures show engine performance only for the first burn. Figure 8a shows the pressure drop induced by the mixing plate (if present), whereas Fig. 8b reports the upstream pressure seen by the

engine nozzle (i.e., the post-chamber pressure p_{post} when the mixing plate is used, and the chamber pressure p_c for the mixerless configuration).

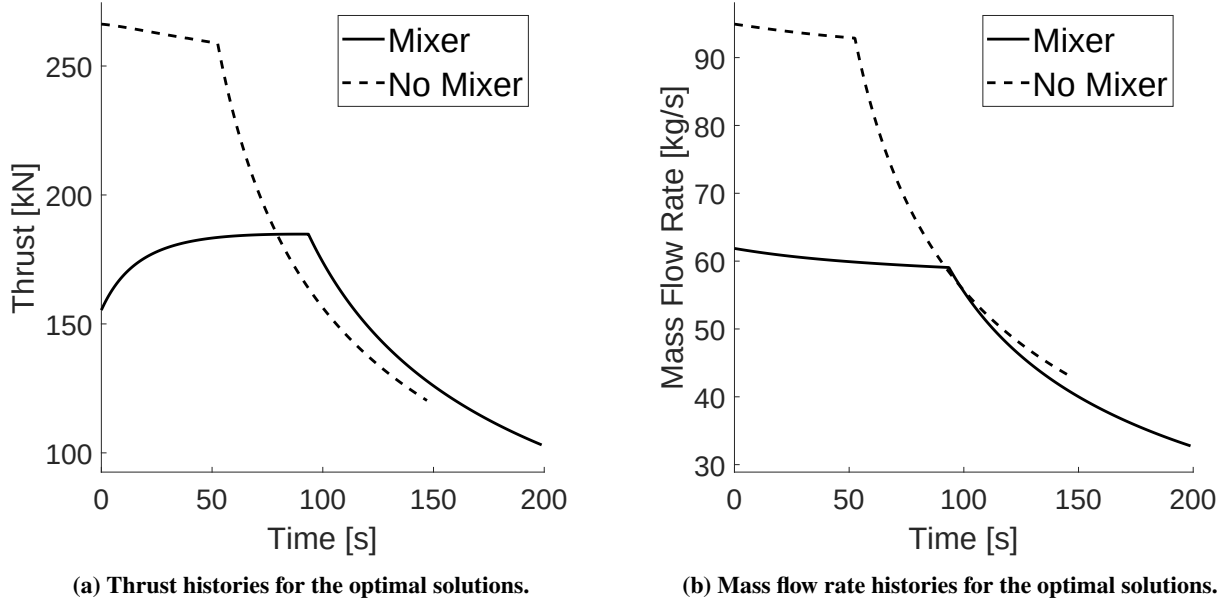


Fig. 5 Time histories of the main propulsion variables for the optimal solutions: (a) thrust, (b) mass flow rate.

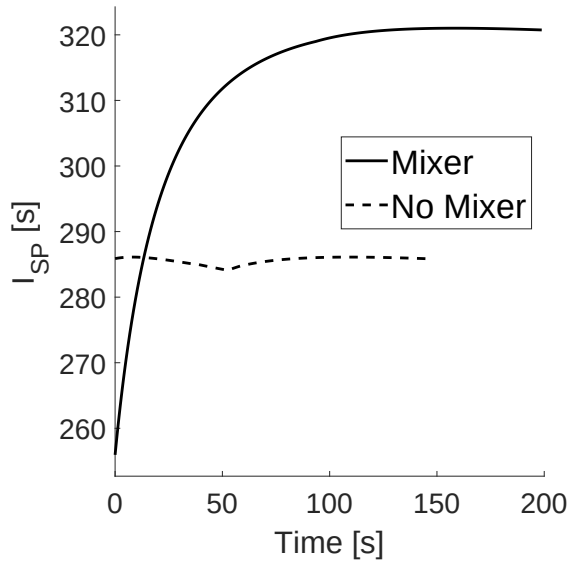
By examining the engine design parameters and their time-dependent performance, several trends emerge.

The optimal mixerless configuration yields $\eta^* = 0.85$, whereas the maximum value predicted by the CRN within the considered design space is $\eta^* = 0.87$. The latter, however, corresponds to substantially higher chamber pressures, while the chamber pressure in this study is fixed at 10 bar. The minimum achievable value is $\eta^* = 0.78$. Accordingly, the optimization seeks a sufficiently high η^* to limit propellant consumption. This drives the mixerless solution toward a larger initial port area $(A_p)_i$ (larger R_g , smaller w) and a longer grain length L_b , which increase the chamber volume and improve η^* .

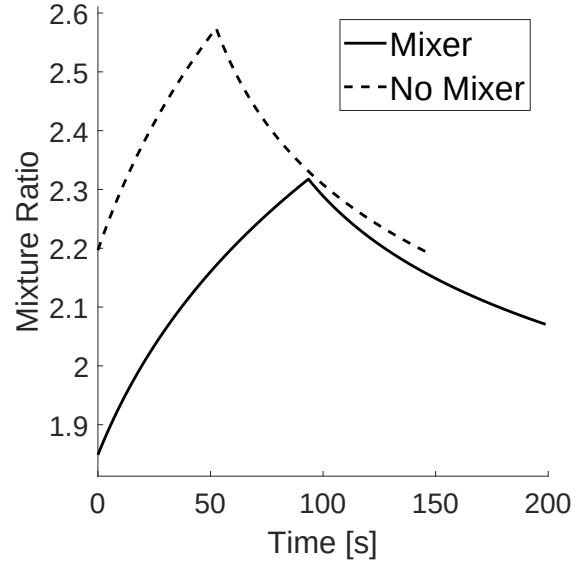
The mixerless optimal design also delivers a higher thrust coefficient, compensating for a characteristic velocity that is lower than in the design employing a mixing plate and post-chamber. This choice, however, results in a heavier nozzle and combustion chamber.

The total propellant consumption is still higher for the mixerless configuration (by approximately 500 kg), although the entire increase is due to additional oxidizer, with a slight reduction in fuel mass. Consequently, the mixture ratio α is consistently higher for the mixerless design.

This trend reflects the trade-off associated with increasing A_p : configurations with a larger mean combustion chamber volume, characterized by a higher $L^* = \bar{V}_c / A_{th}$, tend to exhibit higher η^* , because the extended gas residence time promotes more complete vaporization of the entrained paraffin droplets, consistent with the trend reported in

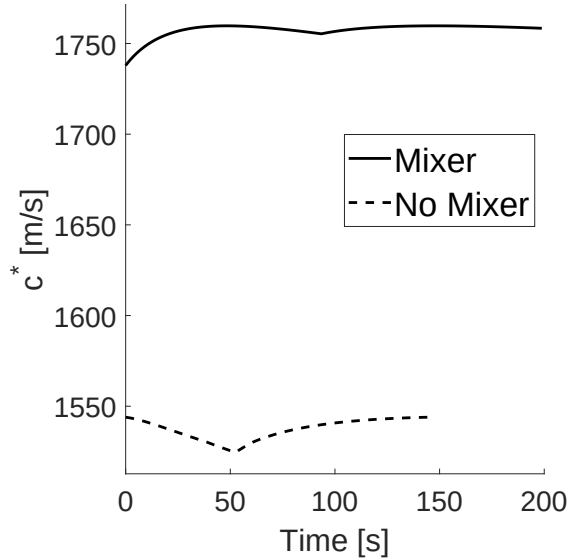


(a) Specific impulse histories for the optimal solutions.

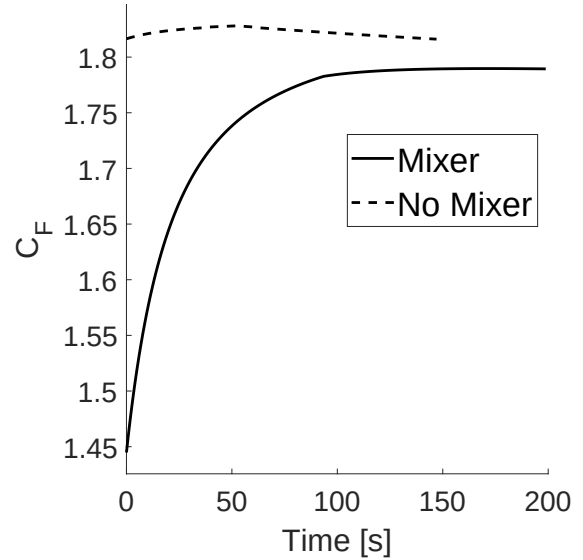


(b) Mixture ratio histories for the optimal solutions.

Fig. 6 Time histories of the main propulsion variables for the optimal solutions: (a) specific impulse, (b) mixture ratio.

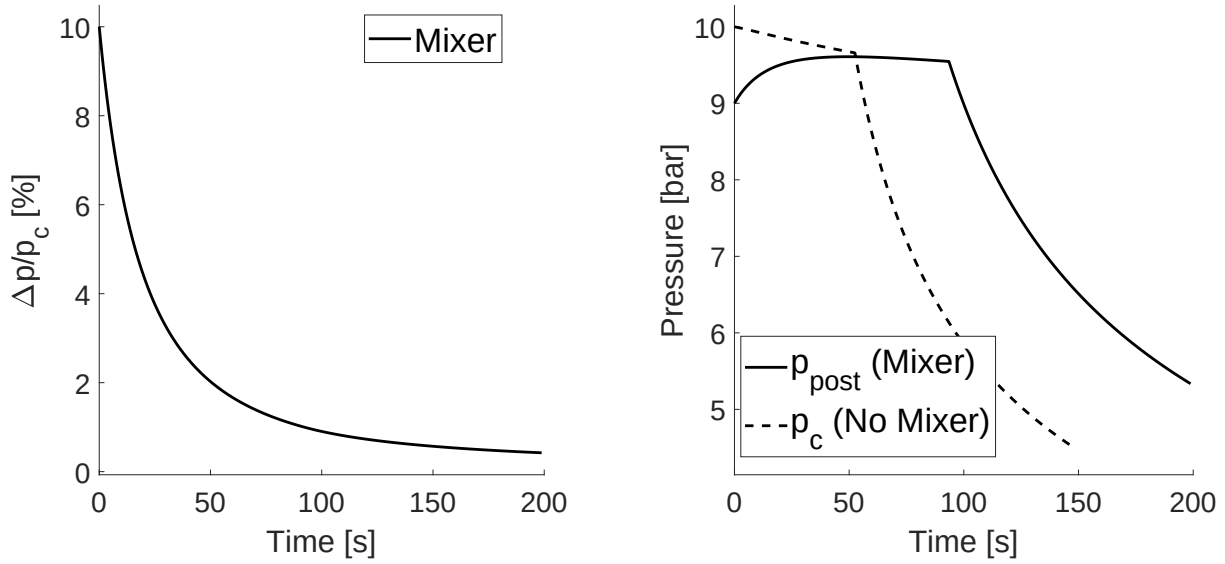


(a) Characteristic velocity histories for the optimal solutions.



(b) Thrust coefficient histories for the optimal solutions.

Fig. 7 Time histories of the main propulsion variables for the optimal solutions: (a) characteristic velocity, (b) thrust coefficient.



(a) Pressure drop history for the optimal solution when mixing devices are employed.

(b) Comparison of post-chamber pressure and chamber pressure histories for the optimal solutions.

Fig. 8 Time histories of the main propulsion variables for the optimal solutions: (a) mixer pressure drop, (b) post-chamber pressure.

Ref. [39] for the SP-1a propellant system. It should be noted that this is a comparison between candidate configurations at their respective mean operating conditions; increasing port area simultaneously reduces the oxidizer mass flux $G_O = \dot{m}_O/A_p$, which enlarges the entrained droplet diameter, reduces the turbulence intensity and acts in opposition to the residence-time gain [53], while also reducing the regression rate. In the design space explored here the L^* effect dominates, but the net direction of the within-burn $\eta^*(t)$ evolution may be propellant- and scale-specific. As a consequence, the total oxidizer mass flow $\dot{m}_O$ increases in order to shift toward the optimal mixture ratio (approximately 2 for the propellant combination considered) and ensure a consistent regression rate despite the larger A_p , thereby improving the ideal characteristic velocity and, once again, reducing the overall propellant consumption. The larger propellant mass flow during the first hundred seconds of the burn, together with larger C_F , chamber pressure, and nozzle throat area, results in a substantial rise in delivered thrust by the mixerless configuration. This, in turn, is balanced by a shorter burn duration (150 s instead of 200 s). It should be noted that longer burn times may increase insulation requirements and nozzle erosion, not included in this work, potentially offsetting part of the payload gain; a dedicated trade-off between payload and burn duration is therefore left to future work.

Looking at the optimal design employing the mixing plate and post-chamber, one can observe that, despite the additional hardware mass ($m_{\text{mix}} = 188$ kg), the overall dry mass is only about 100 kg higher than that of the mixerless architecture. This is almost entirely due to the reduced port area A_p , which causes the nozzle to become lighter and more compact, since the throat area A_{th} scales with the fixed geometric ratio $J = (A_{th}/A_p)_i = 0.5$.

Table 4 Engine design parameters for the optimal solutions.

Design	R_g [m]	w [m]	L_b [m]	$(m_O)_f$ [kg]	$(m_O)_{bBD}$ [kg]	E
Mixer	0.577	0.316	4.181	7022	3821	17.68
No Mixer	0.584	0.279	4.340	7553	3480	17.47

Table 5 Mass budget and performance summary for the optimal solutions.

Design	μ [kg]	m_P [kg]	m_O [kg]	m_F [kg]	m_{dry} [kg]	Φ [kg]	h [km]	η^*
Mixer	2404	10298	7022	3276	1820	2404	700.0	0.96
No Mixer	2068	10736	7553	3183	1718	2068	700.0	0.85

Table 6 Other key parameters for the optimal solutions. In this table m_{feed} is the sum of helium and auxiliary vessel mass.

Design	F_t [kN]	R_{th} [m]	R_e [m]	L [m]	D [m]	L/D	m_c [kg]	m_t [kg]	m_{nz} [kg]	m_{case} [kg]	m_{feed} [kg]	m_{mix} [kg]
Mixer	155.5	0.185	0.776	9.87	1.91	5.16	148	287	288	166	207	188
No Mixer	266.5	0.216	0.902	9.92	1.91	5.18	157	304	366	167	192	-

The significantly improved specific impulse (except during the very initial part of the burn) results from a mixture ratio that remains much closer to its optimal value. As a consequence, the ideal characteristic velocity c^* increases, and the real characteristic velocity also benefits from the higher combustion efficiency ($\eta^* = 0.96$ vs. 0.85). A noteworthy aspect is that, although the total onboard oxidizer mass (and tank mass) is lower in the mixer configuration, the oxidizer mass exhausted before the BD phase $(m_O)_{bBD}$ is actually larger (+9%). This, in turn, causes a slight increase in the feed-system mass (helium plus its pressure vessel) relative to the mixerless case. The optimal value of the grain length is consistent with these trends: the configuration with the mixer selects a shorter grain, since combustion efficiency is ensured by the mixing plate, while the design focus shifts toward reducing the combustion-chamber mass and, in turn, lowering the overall engine dry mass.

Overall, the reduction in propellant mass and the lighter nozzle fully compensate for the additional mass of the mixer and post-chamber, while also enabling a substantial payload increase (+336 kg). All the cited design choices lead to a lower initial thrust level and a longer burn duration, but they also mitigate performance degradation during operation, supported by the extra pressurant mass that helps sustain higher post-chamber pressures over a larger portion of the burn.

V. Conclusions

This work presented a Chemical Reactor Network (CRN) framework integrated into the coupled engine–trajectory optimization of a LOX/paraffin hybrid rocket upper stage. The proposed methodology replaces conventional equilibrium-based performance prediction with a finite-rate chemistry model capable of capturing residence-time effects, incomplete

combustion, and the influence of chamber geometry on reaction progress. The CRN was calibrated using a PSO algorithm against representative experimental data and demonstrated prediction errors within experimental uncertainty, confirming that the model is sufficiently accurate and computationally efficient for repeated evaluations within an optimization loop.

When embedded in the design procedure, the CRN enabled the optimizer to respond directly to the physics of mixing and combustion efficiency. The resulting optimal engine configurations with and without a mixing device diverged significantly, in accordance with expected physical trends. The mixerless solution converged toward larger port areas and longer grains to increase residence time and partially compensate for lower combustion completeness. Conversely, the configuration equipped with a mixing plate is favored by higher characteristic velocity efficiency, enabling a reduction in propellant consumption, a more favorable mixture-ratio history, and ultimately a higher payload mass despite the additional hardware. These differences emerged naturally from the model, highlighting how combustion kinetics and mixing limitations materially influence hybrid engine design when treated consistently within the optimization process.

Overall, the results demonstrate that CRN-based modeling can be used for hybrid rocket engine optimization and it is also beneficial in revealing design trends that cannot be captured when combustion efficiency is prescribed a priori. The methodology offers a robust basis for future investigations aimed at improving the performance, reliability, and physical consistency of hybrid rocket propulsion systems modeling.

To the authors' knowledge, this study represents the first integration of a calibrated CRN into a multidisciplinary optimization framework for hybrid rocket engines. Future developments may include expanding the experimental database used for training, including dedicated hot-fire tests with mixing-enhancing devices, refining the network topology to accommodate different combustion regimes, accounting for nozzle throat erosion, and incorporating a time-resolved evaluation of combustion efficiency directly within the trajectory integration.

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