Nonsteady combustion simulation of 2D hybrid rocket flame

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Abstract

Hybrid rocket propulsion is becoming an appealing option for several types of missions such as suborbital flights or de-orbiting and can be evaluated also for the use in small launchers. Intense investigation efforts are covering several subjects spanning from steady burning rate behavior, to scale-up problems as well as transient behavior. One of the major advantages in the use of this type of propulsion consists of the possibility of thrust modulation during the flight, allowing for flexibility that solid propulsion cannot grant. Existing transient models for solid or liquid propellants cannot be applied due to a consistently different type of combustion involving a turbulent diffusive boundary layer which interacts with a solid fuel surface. The present paper describes the research activity conducted at the Space Propulsion Laboratory of Politecnico di Milano regarding the simulation of steady and unsteady behavior of a hybrid rocket flame in a simplified slab geometry using the *hybridFoam* software. The current unsteady research code is a development of previous versions and is based on the OpenFOAM™ framework library as well as the *reactingFoam* solver. The model considers a solid and a gas-phase region coupled by an interface and resolves Favre-averaged Navier Stokes equations, reduced chemical kinetics, radiation, and heat transfer. The paper addresses the dependence of chemical and physical simulation parameters on the steady and unsteady regression rate and presents a part of the results obtained so far regarding the variation of regression rate as a function of different throttling conditions and rates. The investigation identified some over- and under-shooting phenomena during operations and addressed the role of mass flux and solid phase thermal conductivity in their amplification or damping.

Nomenclature

Greek symbols

α	Thermal diffusivity, m^2/s
α_{rad}	Absorption coefficient - gas
κ	Turbulence kinetic energy, m^2/s^2
ρ	Density, kg/m^3
ε	Rate of dissipation, $N \cdot m/s$
ε_{rad}	Emission coefficient - gas

Roman symbols

A	Pre-exponential of the Arrhenius decomposition law, mm/s
C	Specific heat, $J/(kg \cdot K)$
E_a	Activation energy, J/mol
G_o	Oxidizer mass flux, $kg/(m^2 \cdot s)$
G_w	Radiant heat flux impinging on the wall, W/m^2
h_f	Enthalpy of pyrolysis for solid fuel, J/kg
k	Thermal conductivity, $W/(m \cdot K)$
q	Heat flux, W/m^2
R	Universal gas constant, $8.314 J/(mol \cdot K)$
r	Regression rate, mm/s
t_{tl}	Characteristic time lag of the thermal layer, s
u	Velocity, m/s

Subscripts and superscripts

f	Ref. to solid fuel
g	Ref. to gas phase
s	Ref. to surface

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1. Introduction

A lot of papers have been published in the last decade about hybrid rockets. All of them stress the advantages of this propulsion system, such as engine throttling, multiple ignitions, engine architecture simplicity and cost reduction. These significant advantages are counterbalanced by drawbacks responsible for the poor development of hybrid rocket technology, such as the low regression rate and the poor combustion efficiency. Consequences of these drawbacks are a low thrust level and a lot of unburnt fuel, respectively.

The most important design parameter for a hybrid rocket system is the solid fuel regression rate, which has been largely investigated in these last years. It is the final result of very complex phenomena occurring in a hybrid rocket combustion chamber, where combustion flow fields involve fluid-dynamics coupled with chemical kinetics, heat transfer, turbulence, radiation, fuel surface pyrolysis when conventional polymer-based fuels are used (such as HTPB), or spray atomization, vaporization and combustion when liquid oxidizers are used (such as liquefying fuels, e.g. paraffin-based solid fuels). Typical combustion processes in hybrid rockets involve concurrent phenomena of different physical nature; they are transient, multiphase, multi-domain, three-dimensional, turbulent, obviously reacting phenomena.

The first analytical approaches were developed by Marxman and Muzzy [1] and Marxman and Gilbert [2] in the 1960s, based on the analysis of the reacting turbulent boundary layer characterized by a diffusion-limited combustion process. The models included also, in further developments, radiative effects. The most important result of these approaches is the analytical derivation of the regression rate dependence on the oxidizer flux according to a power law dependency.

Price and Smoot [3, 4] investigated the pressure dependency of the regression rate. Due to the presence of oxygen below the diffusion flame, pressure affects the solid fuel pyrolysis, through heterogeneous reactions at the solid fuel surface. Pressure sensitivity was also observed to increase as the mass flow rate increases. This specific aspect was experimentally investigated in [5, 6], showing the pressure effects on the fuel pyrolysis. The reader should note that an inverse pressure dependency on regression rate was found in [7] though. This latter investigation identified the regression rate behavior to be dependent on the heterogeneous reactions at the solid fuel surface which increase the pyrolysis gas mass flow, enhancing the heat transfer to the solid fuel surface because of the enhanced homogeneous reactions occurring in the gas phase between pyrolysis gases and oxygen.

A model for hybrid rocket flow fields, based on the three-dimensional Reynolds averaged Navier-Stokes equations was developed in [8] using a Lagrangian-Eulerian approach; the liquid oxygen droplets vaporization is responsible for the source terms of the vaporized fuel in the Eulerian gas-phase equations. The 3D flow field is computed in two different motor configurations.

A spray combustion model was developed in [9] for hybrid rocket flow-fields, following an Eulerian-Eulerian approach. Experimental data were used to validate the computational results. Parametric studies were performed to investigate droplet size and oxidizer flow rate effects on the solid fuel regression rate and combustion efficiency.

A computational model for hybrid rocket flow fields simulation was proposed in recent years in [10]. Complete time-dependent Navier-Stokes equations are used; they include turbulence, finite-rate chemistry, radiation and coupling between gas and solid phases. The experimental results by Chiaverini and coworkers [11, 12] are used to characterize the fuel regression rate. Results presented in [10] are two-dimensional and obtained using a quasi-steady assumption; steady-state solutions were obtained to provide the instantaneous burning rates at the operating conditions.

Zilliac and Karabeyoglu [13], starting from Marxman's analytical model pointed out the importance of the thermal flux imbalance at the solid fuel surface, where the coupling between gas and solid phases have to take into account phenomena affecting the surface temperature such as convection, diffusion, radiation, and solid fuel pyrolysis. A regression rate correlation depending not only on GOx, but also on surface temperature, grain length, port diameter, fuel thermo-physical characteristics and flow characteristics was proposed.

The Space Propulsion Laboratory (SPLab) at Politecnico di Milano developed a code [14], using OpenFOAM [15], to perform simulations of the hybrid rocket combustion processes, supported by experimental results. The code uses the Reynolds-averaged Navier-Stokes equation and a chemical kinetics mechanism for HTPB /GOx combustion including six reactions, providing a parametric study on the oxygen mass flow rate dependence.

Two papers have been recently published by Sirignano *et al.* The first [16] develops a model to evaluate the pressure sensitivity to regression rate. This model takes into account the turbulent boundary layer and the diffusion flame to explain the regression rate behavior experimentally observed. Results agree with Risha's *et al.*[7] results. A second paper by this group [17], was recently published about the regression rate prediction of HTPB/GOx formulations. Sensitivities to mass flow rate, combustion chamber pressure and oxygen inlet temperature were investigated. The paper includes also a comparison between two different turbulence models. The performed numerical analysis points out the regression rate sensitivity with respect to each of the investigated parameters, showing the power of the code.

In conclusion, even if many results were obtained so far, the modeling of hybrid rocket combustion processes need to be improved. Research activity was mainly focused on the regression rate modeling, exploiting analytical models and experimental results to describe its behavior. Investigations are needed to improve the modeling of turbulence, chemical kinetic schemes, radiation and multiphase flows to correlate the hybrid rocket behavior to operating parameters. Improvements are especially required under the transient conditions of the hybrid rocket engine, investigated and presented in this paper.

2. Modeling

2.1 Description of the combustion process

The combustion in a hybrid rocket motor consists of the self-sustained thin flame which develops inside a turbulent and reacting boundary layer. A schematic representation of the process considers a gaseous oxidizer which blows over a fuel surface, generally made by a plastic-kind or paraffin-kind material. The burning surface is subjected to a pyrolyzation process which degrades the polymer and produces low molecular weight fuel gases derived from the decomposition of the solid. In this simplified view, neglecting any possible entraining effect due to the use of liquefying fuels, the gases leave the burning surface following a normal direction and mix in cross-flow with the oxidizer to form a boundary layer where turbulent diffusion takes place (fig. 1) [2].

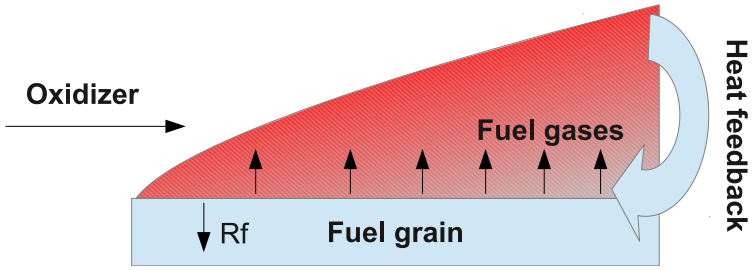


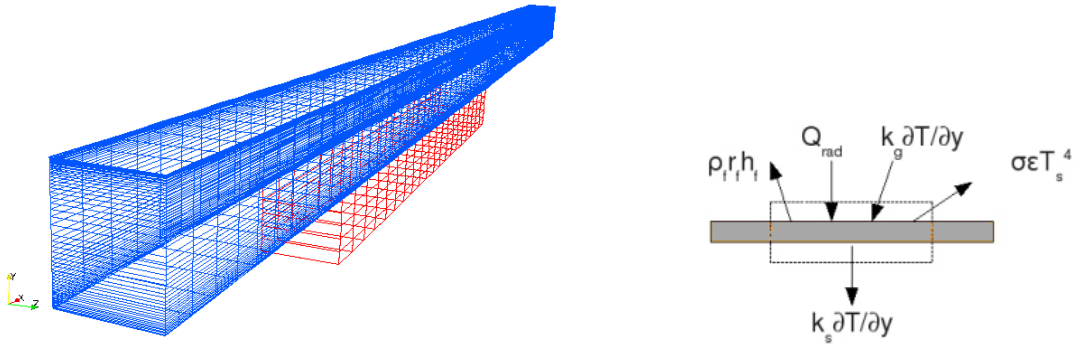
Figure 1: Scheme for the flame typically present in hybrid rockets

Typically, the burning rate in hybrid rockets is small, caused by intermingled physical processes that prevent from high heat feedback from the flame. Proper mixing with the external oxidizer flow must be matched before the ignition of the fuel gases can happen, despite the presence of some heterogeneous reaction at the surface. Due to the diffusive nature of the flame, the composition of the gas phase located close to the burning surface does not have the capability to ignite. Whereas in a solid propellant the flame zone is characterized by a thickness of few hundreds of microns, the hybrid reacting layer can be located some millimeters far from the combustion surface. As consequence of the limited regression rate, a thick temperature profile builds up in the solid phase. The associated thermal lag represents the rate-limiting factor in most of the transient behaviors, being its characteristic time $t_{\mathrm{tl}} = \alpha / r_f^2$ in the order of 0.1-1 s [18]. In that, the solid phase plays a fundamental role requiring proper simulation of its temperature field which must be coupled with the gaseous phase behavior.

The interface between the two phases is represented by the burning surface. Its temperature is determined by the equilibrium of conduction in solid, convection/radiation from gas and pyrolysis which are nested each other. The regression rate is the direct result of the equilibrium temperature on the burning surface since it derives from the pyrolysis of the fuel. Unless a more complex chemical scheme is adopted to include a detailed dynamics in polymer degradation, the reaction rate of fuel decomposition, for simulation purposes, can be assumed to follow a simple zero-order Arrhenius law $r_f = A \exp\left(-E_a/(R\,T_{\mathrm{S}})\right)$ [5, 19, 20]. The direct dependence of Arrhenius data on regression rate implies that the parameters play a fundamental role in steady state operations and regression rate response to throttling [18]. The overall complexity depends on the equilibrium that settles on the burning surface. In fact, an increase in regression rate implies a higher enthalpy request for the pyrolyzation of the fuel which, in turn, acts on the surface temperature and, thus, on pyrolysis rate itself. The regression rate is also responsible for the blowing effect since the injection velocity of the gaseous fuel follows a simple continuity equation where the pyrolyzed mass of the solid phase equals the gaseous fuel production $\rho_f\, r_f = \rho_g\, u_g$. For a matter of simplicity, the fuel is assumed to leave vertically the burning surface.

2.2 Simulation

The simulation of a hybrid rocket flame presented in this paper is performed using a new version of the *hybridFoam* software, a research code grounded on the OpenFOAM^{TM}framework library and developed from the extension of the *reactingFoam* solver [15, 21]. The code considers a 2-D domain split into two main areas representing the solid phase and the gas region, having an interface which represents the combustion surface (fig. 2a). For a matter of simplification, the fuel surface regression is not taken into account, in consideration of the limited rate.



(a) Computational domain. Gas and solid respectively in blue and red color

(b) Energy balance at the interface

Figure 2: Details of the gas-solid computational domain and its coupling

Unsteady heat transfer equation is solved in the solid phase while, in the gas phase, fluid dynamics is ruled by Favre-averaged Navier-Stokes equations, using the Launder-Sharma low Reynolds $\kappa - \epsilon$ model for the closure of the turbulent viscosity. Combustion kinetics is based on a six-reaction compact scheme specialized for butadiene oxidation. The radiative heat flux coming from the gas phase and impinging on the burning surface is evaluated through a P1 Grey model, assuming opaque boundaries. For details on the equations the reader is encouraged to consult the relevant literature [22, 21].

The two computational domains are coupled by an interface which represents the burning surface. Across this boundary, temperature continuity is granted and represents the closure term for the definition of the instantaneous equilibrium between incoming energy from the flame zone, conduction in the solid fuel, radiation, and enthalpy of pyrolyzation of the fuel, which translates into eq. 1, following the scheme reported in fig. 2b.

$$q = \left(k_g \frac{\partial T}{\partial y}\right)\bigg|_{y=0^+} + G_w - \left(k_f \frac{\partial T_s}{\partial y}\right)\bigg|_{y=0^-} - \rho_f r_f h_f - \epsilon_s \sigma T_s^4 = 0 \tag{1}$$

In the balance equation, gradients are evaluated at the inner and outer side of the boundary, the pyrolysis contribution is proportional to the regression rate and the net radiative contribution is dictated by the difference between the radiant flux G_w impinging from the flame to the surface and the re-radiation back to the gaseous domain as well as to the other boundaries. An iterative algorithm grants the solution of the two domains by modifying the interface temperature till eq. 1 is verified within a pre-defined tolerance.

The computational domain represents a simplified version of a 2D slab combustion facility currently operating at the SPLab and is schematically reported in fig. 3. The fuel lamina is 5 cm long and the oxidizer duct is 6 mm thick. The oxidizer O_2 enters from *inlet* face with a constant as well as time-varying velocity following an imposed throttling history and burnt gases exit from the *Outlet* boundary with general zero gradient conditions. The chamber is confined by the walls *MidFlow*,*PreChamber*, and *PostChamber* with constant temperature condition. The *LowerInlet* boundary represents the interface with the solid phase. Fuel gases are injected from this wall along a vertical direction and has a space-dependent temperature which is imposed by the solver and changes locally. The same temperature distribution is found on the coupled solid boundary *Degas*.

3. Results

The dependence of this type of simulation on parameters was the subject of an initial screening. A selection of the most important physical constants was varied in order to evaluate the influence on the steady state average regression rate.

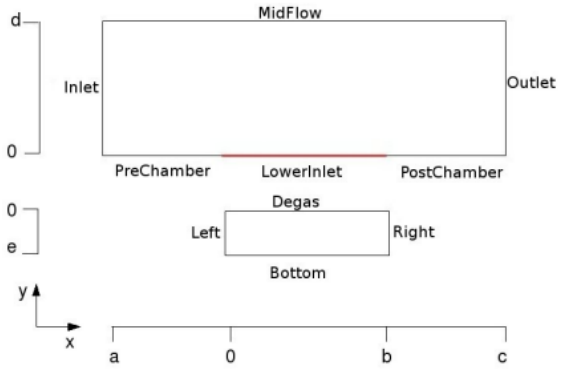


Figure 3: Schematic description of the domain.

	$p[atm]$	$T[K]$	$u[m/s]$
Inlet	$(p_{/x})_{x=a} = 0$	900	fixed value
LowerInlet	$(p_{/y})_{y=0} = 0$	computed	computed
Outlet	2	$(T_{/x})_{x=c} = 0$	$(u_{/x})_{x=c} = 0$
Pre-Post Ch	$(p_{/y})_{y=0} = 0$	900	$u_y = 0$
TopWall	$(p_{/y})_{y\to\infty} = 0$	900	0

Table 1: Standard boundary conditions for the gas phase. Some parameters are computed by the code as part of the solution.

On the basis of such findings, the number of unsteady simulations was shortlisted, giving the priority to the factors that were found more significant, and leaving the rest for a future investigation. In the following lines, a selection of results are reported for both the preliminary analysis and the unsteady findings. Reported regression rate data are space-averaged over the fuel lamina.

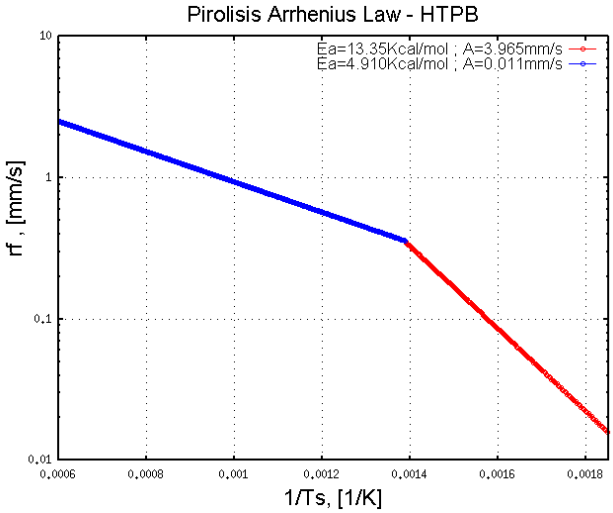
3.1 Preliminary steady-state results

This type of analysis focused on a series of regression rate data obtained in regime condition, once the ignition transient is over and a steady-state condition is reached. Ignition is provided by means of a hot spot located at the head end of the lamina, which impulse is switched off after the flame onset. Finally the system evolves towards its steady state, being inlet mass flow rate and geometry constant. Different runs differ from the value of some relevant simulation parameters which are varied one by one around a standard reference set (fig. 4). The variation of the parameters are chosen, in general, within a range of practical interest.

The first investigation regarded the variation of the thermal conductivity for the fuel polymer. The doubling of k_f (from 0.14 $W/(m \cdot K)$ for HTPB to 0.25 $W/(m \cdot K)$ of paraffin) shows a marked influence on burning rate which can be altered even up to about 30% in the investigated range. Whereas for low mass fluxes a linear and rather limited dependence between r_f and k_f is found, for higher value of G_o a more complex dependence is evidenced, mainly for low k_f (fig. 5). As visible from the ignition transient, under the tested conditions the steady state is reached before 10 ms, regardless of the value of k_f, showing a minimal overshoot mainly dependent on the igniter action which has a duration in the order of 1 ms.

Test variation on fuel specific heat should be read in conjunction to the test on k_f since the ruling parameter of heat transfer in the solid phase consists of the diffusivity $\alpha_f = k_f/(\rho_f \cdot C_f)$. Being ρ_f kept constant, a variation of C_f and k_f rules α_f. However, the specific heat of candidate polymers for this type of application do not change significantly, thus reflecting into a limited dependence of the regression rate within the tested range (fig. 6a).

Influence of gas-phase radiation properties was also addressed. In the simplified view of this model, emissivity is kept constant regardless the composition. It is likely that, depending on soot presence, real emissivity may grow. Different cases were considered, from the current standard value $\varepsilon_{rad} = 0.5$ to almost black body emission. However, it was found that the strongest variation on steady regression rate was as high as +10% under the tested operating conditions.

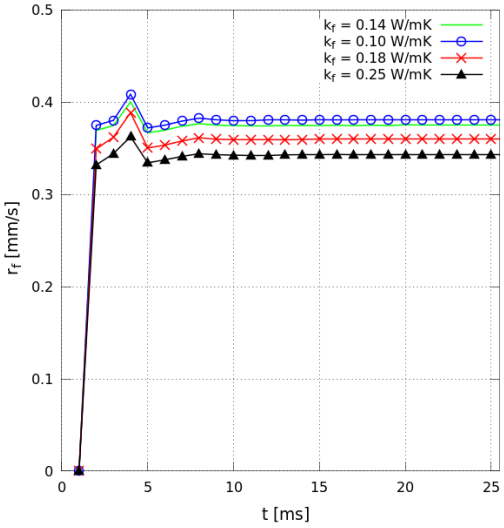


(a) Kinetics of pyrolysis for HTPB

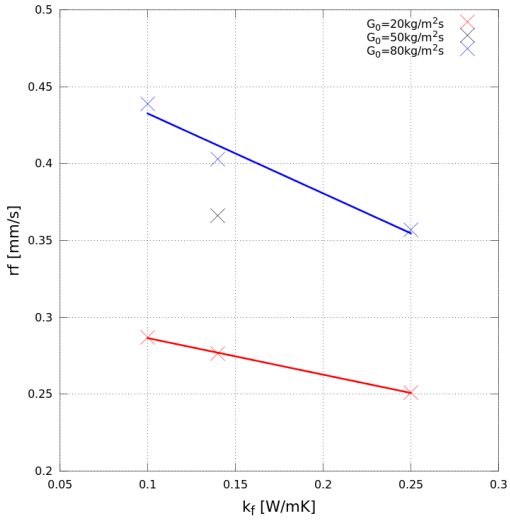
Constant	Standard value	unit
ρ_f	920	kg/m^3
k_f	0.14	$W/(m \cdot K)$
C_f	2000	$J/(kg \cdot K)$
α_{rad}	0.5	
ε_{rad}	0.5	
h_f	1.81	MJ/kg

(b) Simulation parameters

Figure 4: Standard parameters for the solver

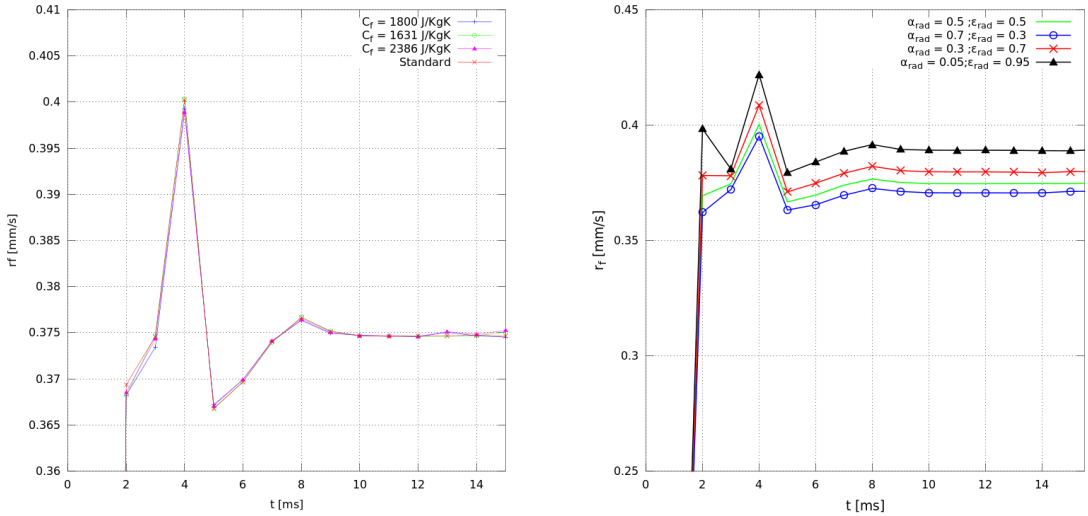


(a) Ignition to steady state



(b) Summary of tests on k_f

Figure 5: Tests on conductivity. Inlet speed: 60 m/s; pressure: 2 atm.



(a) Solid fuel specific heat

(b) Gas phase emissivity

Figure 6: Effect of specific heat and emissivity. Inlet speed: 60 m/s; pressure: 2 atm.

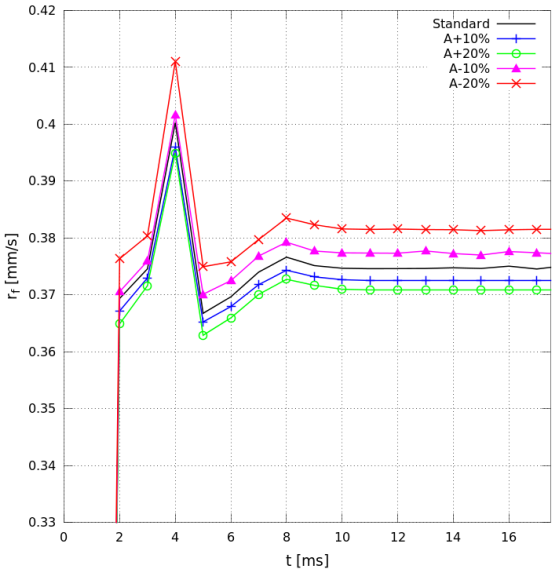


Figure 7: Effect of Arrhenius pre-exponential constant. Inlet speed: 60 m/s; pressure: 2 atm.

Significant results were obtained for the analysis of regression rate dependence on Arrhenius parameters. Only the variation of the pre-exponential term was considered. Data were found to follow an inverse trend where an increase of A leads to a reduction of r_f and *vice versa*. At a first sight this result might appear a nonsense due to the fact that Arrhenius law rules the regression rate. However, the interpretation should consider the problem in its whole. The increase in regression rate is also leading to an augmented enthalpy requirement for pyrolysis and a higher blowing effect which inflates the boundary layer. Thus, under some conditions, the heat feedback can somehow be reduced causing a contraction of the r_f. It follows that the result should be not be considered as a general indication but it characterizes the equilibrium among all heat contributions on the burning surface under tested conditions.

3.2 Transient results

The simulation of the transient behavior was accomplished by supplying variable mass flow rate at the inlet. The code started from a steady-state combustion condition, after the oscillations due to ignition transient were damped. The throttling ratio was maintained constant in the range ±50% of the initial G_o for all the tests whereas different time lapses (from 1 to 5 ms) were considered in order to modify the derivative. The model was tested under the following maneuvers:

- steady state to +50% to steady state (1:1.5:1);
- steady state to -50% to steady state (1:0.5:1);
- double throttling from +50% to -50% (1:1.5:0.5:1);

An example of the G_o variation in time is reported in fig. 8 while fig. 9 collects some representative results of throttling response as a function of solid phase conductivity. Due to the transient nature of the monitored variables, the ratio between instantaneous and steady state regression rate is reported.

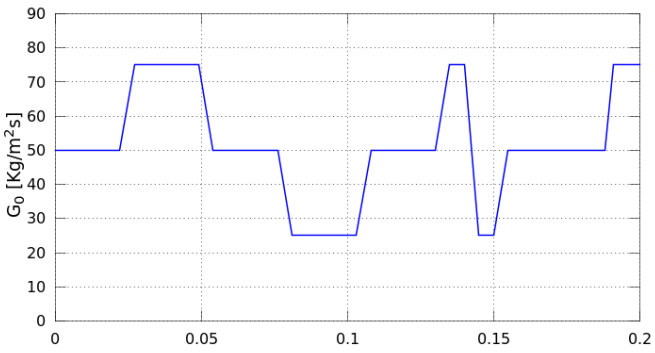
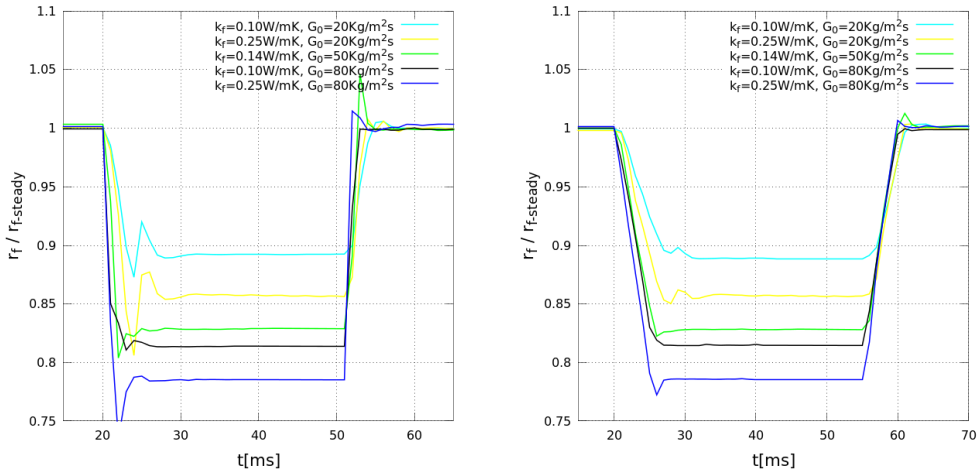


Figure 8: Example of mass flow variation for transient tests

During the step-down throttling maneuver 1:0.5:1 an undershoot followed by an overshoot of the average regression rate could be observed for the fastest transient case. The elongations could rate some percentage of the steady state value. However, these transient adjustments of the regression rate turned into a steady condition after less than 10 ms. In the case of the slowest maneuver, all events were damped.

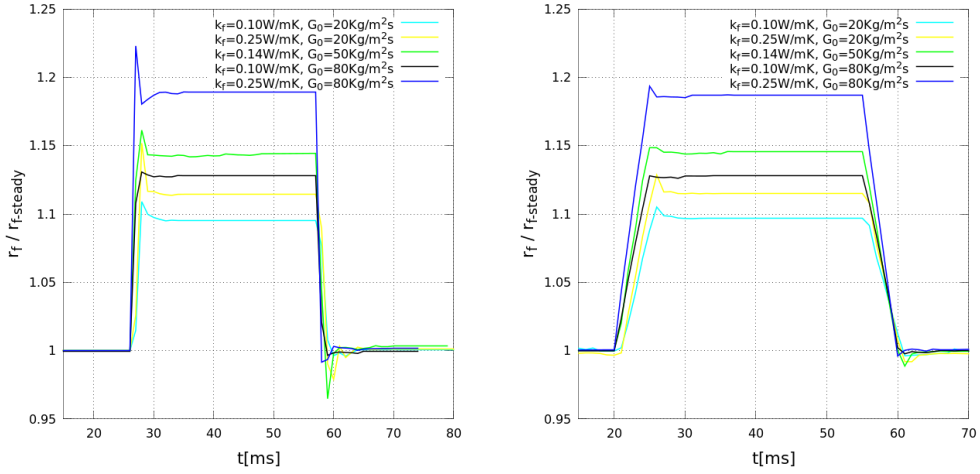
For the step-up throttling 1:1.5:1, a sharp overshoot can be observed for the fastest maneuver. The elongation is rated about the same quantity of the undershoot observed for the step-down case but, in the present maneuver, the regression rate converges back to a steady condition without oscillations.

In the case of the double throttling 1:1.5:0.5:1, the scenario is more complex. Maneuvers and stabilization periods have the same length. That is, in most cases the overshooting is not yet stabilized back to steady state when the following maneuver is performed. Moreover, the central throttling from +50% to -50% effectively doubles the rate of change for G_o. For all these reasons, the plot is not symmetric. The answer to the down-step is pronounced and produces consistent undershoot and deformation of the curve in the slowest case. On the opposite side, for fastest transient, curves do not have time to come in a steady-state condition and the answer is quite deformed. Moreover, once back to the initial condition, a final minor oscillation is still present and fades out.



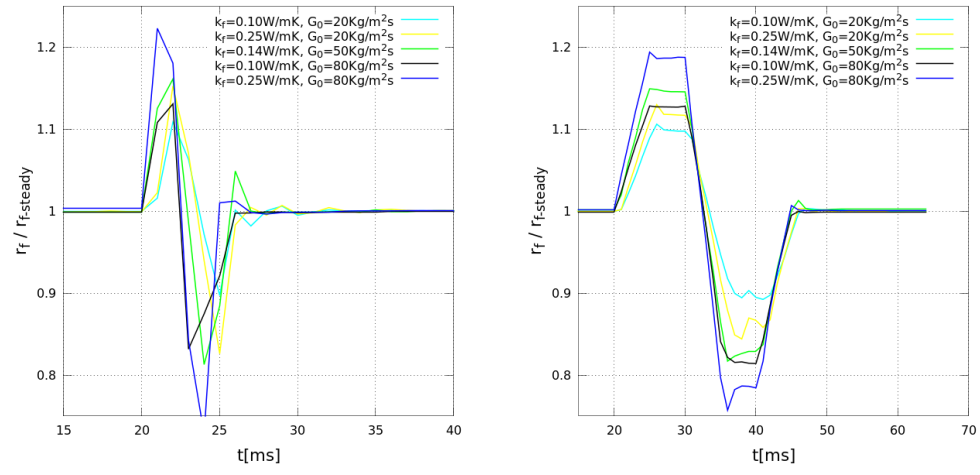
(a) 1:0.5:1 - 1 ms

(b) 1:0.5:1 - 5 ms



(c) 1:1.5:1 - 1 ms

(d) 1:1.5:1 - 5 ms



(e) 1:1.5:0.5:1 - 1 ms

(f) 1:1.5:0.5:1 - 5 ms

Figure 9: Response to transient mass flux. Throttling ratio and maneuver time are reported in captions.

4. Discussion

Looking at this snapshot of steady state and transient results, the dependence on mass flow rate conditions and thermal conductivity is worth of consideration. As expected, the throttling speed is an important parameter since in all the cases with the slowest maneuver (execution time 5 ms) only minor over- or undershooting were registered. Under a faster throttling condition (execution time 1 ms), the deviation from the theoretical behavior can be as high as 10%. This influence is in line with the presence of a thermal layer featured by its own inertia in the solid phase. Regardless of the transient, it could be observed that higher initial mass flux confers to the system a higher sensitivity and the process is prone to evident deviations from an ideal smooth behavior.

Some more considerations and supplement of investigation should be devoted to the influence of k_f on both steady state and transient behavior. To date, from throttling results it seems that the system is more sensitive to mass flux variations in presence of a higher conductivity. This is translated into both the presence of peaks which further damp as well as into higher r_f variation once the curve is stabilized into the new inlet condition. However, this appears to be in contrast with steady state analyses and require further refinement.

It was also interesting to observe that, in the range of potential variability, fuel specific heat does not play a role in the definition of the burning rate whereas gas phase emissivity and Arrhenius parameters limit their influence to less than 10%.

5. Conclusion

This paper has presented some preliminary results obtained in the analysis of the transient behavior for a hybrid rocket flame. The code introduced several simplifications such as steady burning surface (no mesh motion considered), constant specific heat of the solid phase and simplified 2D slab geometry. The investigation regarded both a sensitivity study for some of the simulation parameters and and investigation of the transient behavior from a reference condition. The analysis revealed that, if throttling is accomplished with a proper rate, r_f oscillations present over or undershooting and the magnitude of the effect is more pronounced for higher initial mass fluxes. The process is fast and stabilizes within few milliseconds. The role of conductivity was also addressed but a supplement of investigation is required.

The code has demonstrated to operate correctly in a transient situation. However, the effect of only few parameters was considered on throttling response and should be completed. The investigation should also consider the coupling with a nozzle. Given the importance that radiation can have in presence of some kinds of hydrocarbon fuels, a different kinetic scheme should be considered, if soot formation and relevant effects on the burning surface have to be included. From the numerical point of view, the code requires a tuning. Despite some work has been performed for its optimization which cut the simulation time by a factor of 10, the current wall-clock time for the execution of one case prevents the use of the code to more extended geometries.

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