Numerical approaches for the analysis of hybrid rocket flowfields

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The intrinsic properties of hybrid propellant rockets in terms of performance, simplicity, safety, reliability, low development cost, reduced environmental pollution, and flexibility, make them as one of the envisaged future generation propulsion systems [1]. Nevertheless, the hybrid engine development has not achieved the same level of maturity as solid and liquid traditional systems. Therefore, as the new international attention to hybrid propulsion points out, the hybrid system design needs a better understanding of the physico-chemical phenomena that control the combustion process and of the fluid dynamics inside the motor [1, 2, 3]. The knowledge of the complex interactions among fluid dynamics, solid fuel pyrolysis, oxidizer atomization and vaporization, mixing and combustion in the gas phase, particulate formation, and radiative characteristics of the gas and the flame can only be improved by combined experimental and numerical research activities. Similar considerations can be made regarding the ablation process of the nozzle thermal protection system (TPS). The numerical study of the flow in the combustion chamber and in the nozzle of a hybrid propellant rocket requires the ability to describe adequately the interaction between the reacting flow and the solid surface through suitable gas-surface interaction (GSI) modeling.

In a classical hybrid propellant rocket, the liquid or gaseous oxidizer injected into the ports of solid fuel grain (typical fuel is HTPB, Hydroxyl-Terminated Poly-Butadiene) reacts in the combustion chamber with the pyrolysis gas, which is produced on the surface and diffuses into the boundary layer, forming a turbulent diffusion flame. The convective and radiative heat flux from the flame, in turn, provides the energy needed for the pyrolysis process of solid fuel. It is evident that the fuel regression rate is governed by the interaction between these different processes. The solid fuel in a hybrid rocket regresses slowly making in fact necessary to use a large fuel surface exposed to hot gas to get the mass flow rate required by the motor design. The solid fuel regression rate and its dependence on various operating conditions is therefore of basic importance in the design and development of hybrid rockets. Classical studies on hybrid propulsion are based on simplified models of the boundary layer to derive the heat flux to the surface of the solid fuel and, therefore, its regression rate [4]. However, this simplified analysis can not take into account many of the complex chemical and physical interactions between the various processes, such as the effect of changes in operating conditions, chamber pressure, radiation and finite-rate chemistry, making necessary the development of more advanced models based on computational fluid dynamics (CFD) to improve prediction and analysis capabilities for such propulsion systems. A common approach is therefore that of solving the Reynolds averaged Navier-Stokes (RANS) equations, with suitable turbulence closure models. In particular, there is an interest in obtaining steady-state solutions by solving RANS equations, as justified by the fact that chemical and fluid-dynamic time scales are much faster than the regression rate time scale. Therefore, a valid approach to study the hybrid rocket internal ballistics can be that of simulating the flow at different times thus considering different chamber geometries [5]. However, in addition to the equations of motion, the various physical phenomena and chemical characteristics of these propulsion systems have to be suitably modeled: the coupling between the gas and solid phase based on mass and energy balances, the fuel surface pyrolysis and regression rate, the finite-rate chemistry to describe the combustion process, and the turbulent diffusion of oxidizing species and of the pyrolysis gas.

The objective of this study, which is carried out within the framework of an Italian project [6], is the simulation of the flow inside the combustion chamber and nozzle of a hybrid rocket. In the present study, a simplified kinetic model is adopted, i.e. a comprehensive combustion model, based on a small number of reaction steps [7]. In fact, a detailed model of chemical kinetics is very complicated and, in this case, could involve more than 50 chemical species and hundreds of elementary reaction steps [5]. A simplified kinetic model reduces the computing time by reducing the number of species involved in the overall reaction and is therefore the most efficient way to achieve the goal of a complete modeling of physical-chemical processes within a hybrid rocket and therefore to validate the simulation model. Regarding the process of solid fuel pyrolysis, it can be described by semi-empirical models (such as those proposed in [8, 9]) in which the rate of pyrolysis is expressed through an Arrhenius type relationship where the unknowns are the solid fuel surface temperature and regression rate. To obtain the solution of the flow field it is therefore necessary a coupling between the solid and gas phase by introducing suitable boundary conditions. This boundary condition on the solid fuel surface requires mass and energy balances, which, together with pyrolysis and gas-phase combustion models, yield a coupled gas-surface solution. The surface energy balance involves different contributions to wall heat flux: the convective heat flux related to temperature gradient, the heat flux related to diffusive gradients of concentration, the possible radiative heat flux, the conduction heat flux in the solid phase, and the pyrolysis heat flux due to mass injection in the flow field. A similar mass balance can be defined for each chemical species considering the diffusive flux, the convective flux due to mass injection, and the source term due to thermal decomposition during the pyrolysis process. The model for the boundary condition developed in [10, 11] for the ablative thermal protection is also based on surface mass and energy balances and this model is extended here to the case of solid fuel pyrolysis. Finally a model has to be introduced to describe the heat conduction within the solid fuel. Similarly to what done for the analysis of ablative thermal protection systems, the assumption of steady-state thermal field within the fuel can be made, which is considered appropriate for the hybrid rocket conditions [5].

The numerical simulations are carried out by solving Reynolds averaged Navier-Stokes equations for single-phase multicomponent reacting flows, including the required sub-models in order to describe: homogeneous combustion in the gas phase, fluid-surface interaction in the combustion chamber (solid fuel pyrolysis model) and fluid-surface interaction in the nozzle (material thermochemical ablation model). The resulting set of Reynolds Averaged Navier-Stokes equations for turbulent chemically reacting flows is solved by two different approaches: one, referred to as FNS, solves the full system of time-dependent equations up to reach a final steady solutions, the other, referred to as PNS, solves the steady-state set of equations suitably simplified to solve them by a space-marching approach.

The FNS (Full Navier-Stokes) approach has been successfully used for the analysis of different liquid and solid rockets problems [12]. In particular, hybrid rocket nozzle flowfields and thermal protection system behavior has been recently studied [13]. Sample results in terms of erosion rate and nozzle wall temperature of these aforementioned studies are shown in Fig. 1. In particular, the nozzle flowfield and wall TPS behavior has been studied for different combinations of fuel and oxidizer. Results have shown that erosion rate levels are 1.5 up to 3 times that of a comparable aluminized solid fuel, depending on the choice of the oxidizer, as shown in Fig. 1. The type of oxidizer, in fact, can significantly influence the erosion rate, with high-oxygen content oxidizers such as oxygen and nitrogen tetroxide showing the highest values. On the contrary, the choice of the fuel has not shown any significant effect on the erosion rate level. The oxygen content in the oxidizer is not the only parameter affecting the erosion rate level, as the flame temperature and the type of oxidizing species present in the exhaust gas also play an important role. Erosion rate in hybrid rockets is also shown to be significantly affected by O/F shifting. Despite the reduction in flame temperature, oxidizer-rich conditions produce only a limited reduction in the throat erosion rate due to combined effect of the increased erosion contribution by molecular oxygen and its exothermic reaction with graphite. On the contrary, fuel-rich conditions can significantly help in reducing the erosion rate level.

The PNS (Parabolized Navier-Stokes) approach, relies on the hypothesis of neglecting the diffusive terms in the axial direction [14, 15]. With this hypothesis the solution can be obtained marching in the space once the axial pressure gradient is suitably evaluated. The present approach has been successfully used in the study of supercritical fluid flows in heated channels and is extended here to the case of hybrid rockets combustion chamber. Preliminary results relevant to the mixing of fuel and oxidizer are summarized in Fig. 2. The test case is a straight channel of length $L = 66$ cm with a constant circular cross section with a diameter of $D = 7$ cm, which is schematically reported in Fig. 2(a). The inflow is pure oxygen, with a temperature $T = 1000$ K, whereas a mass flow rate of methane at $T = 3000\ K$ is continuously added along the side wall. Smooth solutions are obtained, thus demonstrating the good response of the numerical scheme with respect to the transversal inflow, as shown by results in Fig. 2(b) in terms of methane mass fraction: at the chamber inlet no methane is present in the whole cross section; further downstream a mass fraction gradient is clearly established and methane mass fraction goes from a unitary value at the wall (where methane is injected) to a null value at the edge of the mixing layer.

Simulations on hybrid rocket combustion chamber with both approaches are being carried out on the geometry and operating conditions of the aforementioned research project, which are being defined in these days and for which also experimental tests are planned [6]. Results of simulations will be presented in the final paper.

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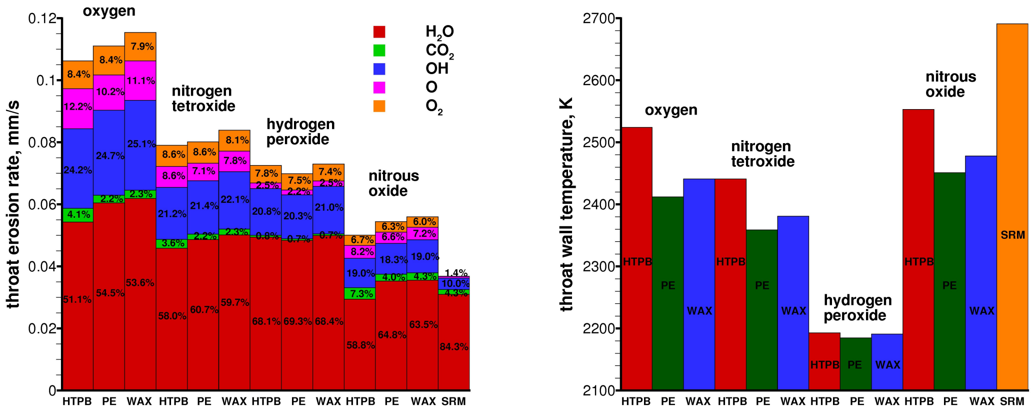
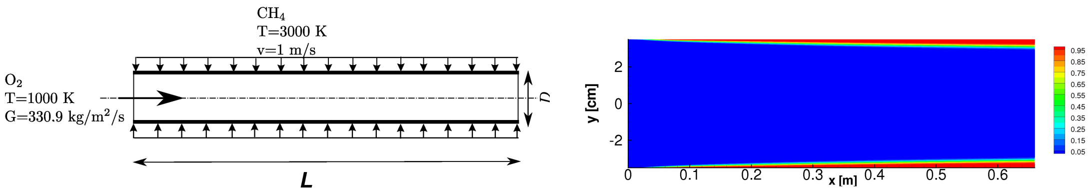


(a) Erosion rate and oxidizing species contributions

(b) Wall temperature

Figure 1: Throat erosion rate and wall temperature for various propellant combinations compared with an aluminized solid rocket propellant (SRM)



(a) PNS preliminary test case CH_4 molar fraction

(b) CH_4 molar fraction

Figure 2: Test case boundary conditions and computed flowfield for the preliminary test case carried out with the PNS solver