Consistent flamelet-based turbulent combustion modeling for liquid rocket engines

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Abstract
In this work we present a consistent flamelet-based framework for turbulent combustion modeling in liquid rocket engines. This approach is based on the low-Mach number approximation of the governing equations and on the tabulation of all the thermochemical properties by means of steady laminar flamelets. The proposed framework features the possibility to accommodate, in a computationally efficient manner, real gas thermodynamics and to account for non-adiabatic combustion in the presence of wall heat transfer. Such capabilities are tested separately on two well-established experimental configurations consisting in methane-oxygen flames at elevated pressures, by means of unsteady Reynolds averaged Navier Stokes simulations.

Introduction
Space propulsion is one of the most extreme applications of energy conversion by means of combustion since it usually occurs at high pressure, such as those encountered in liquid rocket engines (LRE) combustion chambers. For these devices the most significant technological trend over the years was increasing the thrust levels, which directly promoted a significant increase of the operating chamber pressure in order to improve performances and allowing engines to remain reasonably sized [1].

This rise in the operating pressure causes at least two technological drawbacks. Firstly wall heat transfer in combustion chamber of a LRE scales almost linearly with pressure, thus causing additional loads for both structures and cooling system. Secondly, typical operating pressures are above the critical pressure of a large part of the propellant combinations which are typically used by LRE therefore they will most likely behave like complex fluids rather than an ideal gas or liquid and poses serious challenges to the physical understanding and the numerical modeling [2].

Despite the great experimental and theoretical/numerical effort in the past decades, supercritical mixing and combustion processes in LRE combustion chambers are still to be completely understood [3], motivating a substantial research effort toward reliable computational fluid dynamics (CFD) tools.

In this contribution we present a consistent framework to simulate the subsonic part of LRE combustion chambers, i.e. the injector plate near field where the mixing and combustion occur in order to achieve elevated combustion efficiencies [1].
This consideration in conjunction with recent direct numerical simulations results [4] motivate the adoption, in this context, of a low-Mach number approximation of the governing equations. In the low-Mach number limit, flamelet based tabulation methods for turbulent non-premixed combustion are well-posed [5], and provide a properly filtered/averaged treatment of a real fluid equation of state (EoS) [6]. The ensuing flamelet generated thermodynamic manifolds can be extended to account for non-adiabatic flows due to wall heat transfer. Although non-adiabatic tabulation strategies have been successfully developed in the context of premixed combustion, the inclusion of enthalpy losses for high pressure non-premixed flames is less studied. A pragmatic approach to this issue is to adopt enthalpy defect methods developed for sooting non-premixed flames which are influenced by radiative heat transfer [7].

The mentioned key capabilities, namely the efficient inclusion of real gas EoS and wall heat transfer, are separately assessed by means of two LRE-oriented experimental configurations featuring methane-oxygen flames at elevated pressures. In particular the inclusion of real gas effects is tested on a reference cryogenic liquid oxygen (LOx) and gaseous methane (GCH4) using the configuration and thermodynamic conditions of the G2 test case of described in [8]. On the other hand, the modeling of non-adiabatic effects is tested simulating a model gaseous oxygen (GOx)-GCH4 single injector combustion chamber [9] for which experimental results are available in terms of wall heat transfer at the chamber wall. All the simulations presented in this work are based on an unsteady Reynolds averaged Navier Stokes approach in order to capture, with reasonably computational costs, the low frequency unsteadiness of the combustion process.

**Theoretical and numerical framework**

Flamelet based combustion models for non-premixed combustion lay the foundations on the assumption that a turbulent non-premixed flame can be treated as an ensemble of thin laminar diffusion flames, namely the *flamelets*. This flamelet assumption is justified as long as the chemical reaction region remain thin compared to small scales vortices [10]. These requirements are usually met by high pressure flames in both subcritical and supercritical pressure environments [11].

The main advantage of such formulation lies in the fact that, irrespective of the thermodynamic model used, laminar flamelet solutions are obtained as steady state solutions of one dimensional laminar problems (flamelet equations or counterflow flames) at a given constant thermodynamic pressure $p_0$ [5]. The ensuing laminar flame structures, which can be referred to as thermodynamic manifolds, can be expressed, for non-adiabatic non-premixed flame, as:

$$
\psi = \psi(Z; \chi_{st}, \phi_H)
$$

where $\psi$ is a generic thermodynamic variable, $Z$ is the mixture fraction, $\chi_{st}$ is the scalar dissipation rate of the mixture fraction at stoichiometric conditions and $\phi_H$ is the enthalpy defect. The latter is defined as the difference between the actual or
transported enthalpy and the enthalpy of an adiabatic mixture characterized by the same value of the mixture fraction [7].

The Favre averaged mean values which are needed by the CFD solver are obtained through multi-variate probability density function (p.d.f.) which represent the turbulence-chemistry interactions at a sub grid scale (SGS) level:

\[
\tilde{\psi} = \int_{-\infty}^{+\infty} \int_0^1 \int_0^1 \psi(Z, \chi_{st}, \phi_H) p(Z, \chi_{st}, \phi_H) \, dZ \, d\chi_{st} \, d\phi_H
\]

where the joint p.d.f. is usually approximated, assuming statistical independence, using Bayes theorem as the product of single-variate p.d.f. of the variables. The three ensuing p.d.f.s are then modeled using a presumed p.d.f. approach, with a beta-p.d.f. for the mixture fraction distribution, a log-normal p.d.f for the scalar dissipation rate and Dirac delta for the enthalpy defect [7]. In particular the beta-p.d.f. is constructed starting from the first two statistical moments of the mixture fraction, namely its mean and variance, the latter represents the unresolved SGS fluctuations of \( Z \). As a result the full thermodynamic manifold, composed of the mean quantities can be expressed, with the following expression, as a look-up table which can be efficiently accessed during the simulation [12]:

\[
\tilde{\psi} = \tilde{\psi}(\bar{Z}, \bar{Z}''^2, \bar{\chi}_{st}, \bar{\phi}_H)
\]

Noteworthy of mention is the fact that this manifold includes a consistent averaging of the EoS via density tabulation [5,6]. It is important to remark that the generation of thermodynamic manifolds is strictly case dependent since it is constructed starting from the thermodynamic boundary conditions of the test case. In this work we use the low-Mach URANS solver FlameletPimpleSMOKE [13] developed in the context of the open source OpenFOAM framework which implements a classical non-adiabatic steady flamelet formulation [12]. It solves the Favre averaged RANS equations for mass and momentum coupled with three additional transport equations for the mean mixture fraction its variance and the mean enthalpy. In order to access the thermodynamic manifold the scalar dissipation rate and the enthalpy defect are obtained through an algebraic models [12,13]. The system is closed with a standard two equation \( k-\varepsilon \) turbulence model with the adoption of wall functions in order to blend the grid requirements imposed by boundary layers [14].

**Transcritical flame**

The reference LOx-GCH4 flame used in this work is taken from the G2 case of the Mascotte test bench at ONERA described in [8]. The configuration consists in a prismatic test chamber (dimensions: 50x50x400 mm\(^3\)) maintained at an operative chamber pressure of \( p_0 = 56.1 \) bar. This pressure level is supercritical for both the fuel and the oxidizer, which is injected by the central part of a co-axial injector in a transcritical state (\( T_{LOX} = 120 \) K) of elevated density and viscosity, while methane
is injected by the outer part of the injector in a supercritical state \(T_{\text{GCH}_4} = 288\, \text{K}\) of lower density and, as a result, greater injection velocity. The URANS simulation uses a 2D axy-symmetric computational domain, whose dimension have been chosen to reproduce the hydraulic diameter of the chamber, similarly to other RANS studies [15]. The computational domain is discretized with 30000 finite volumes, which have shown to correctly capture the main flow fields patterns. The case dependent thermodynamic manifold, which is adiabatic in this simulation, is generated using the OpenSMOKE++ [13] framework and the GRI 3.0 chemical kinetic mechanism. Real fluids effects are including via multi-fluid-mixing (MFM) model [16], that has been recently validated for this case [6].

![Figure 1. Structure of the LOx-methane flame of the G2 case [8]. Qualitative comparison between time averaged OH mass fraction of the simulation (top half) and the averaged experimental Abel transformed OH emission image (bottom half).](image)

The top half of Fig.1 displays the structure of the cryogenic flame in terms of time averaged OH mass fraction, which has been obtained averaging the URANS simulation. The bottom half of the same figure display the averaged experimental OH emission, Abel transformed image, taken from [8]. The numerical result are in good qualitative agreement with the limited experimental informations available. The simulation capture well the main morphological features of the flame, which are the flame length and its abrupt termination after a sudden expansion, in accordance with recent LES results [17].

**Wall heat transfer**

Along with the mixing and combustion at high pressure, another key aspect of LRE design is the characterization of combustion chamber wall heat loads. The latter determines both the sizing and operative parameters of the regenerative cooling system and is generally tackled separately from the mixing and combustion of the propellants. In this context, the numerical simulation of both the mixing/combustion phenomena and wall heat loads can provide useful physical insights on the reacting flow field in the combustion chamber and, more practically, actively supports the design process. For these reason we perform numerical simulations focused on wall heat loads of a single-element GCH4/GOX experimental configuration. This experimental configuration has been recently described by Celano et al. [9], and provides...
measurements of wall heat transfer under conditions relevant for LREs. The operative pressure is 20 bar and GOX and GCH4 are respectively injected at 278 K and 269 K. Following [7] the non-adiabatic thermodynamic manifold has been discretized with at least 100 enthalpy defect shelves in the flamelet libraries.

**Figure 2.** Left panel: instantaneous temperature representative iso-surfaces inside the single element combustion chamber in the 3D URANS simulation. Right panel: Axial distribution of heat flux along the chamber wall. Symbols represent the experimental values using two different approaches, continuous and dashed lines denote, respectively 2D and 3D results.

In this case we have conducted both 2D and 3D simulations with similar grid resolution (smallest finite volume with characteristic dimension of 0.1 mm) and flamelet libraries. An instantaneous temperature field overview is shown in the left panel of Fig.2. The results in terms of wall heat transfer time averages are displayed in the right panel of Fig.3 for both 3D and 2D URANS simulations. The trends show that both the simulations well-capture the experimental results, even if some differences can be observed between the 2D and 3D profiles. Since the resolution of the computational grid is similar the observed differences can be attributed to the interaction between the conical shape of the diffusive flame in the injector near field region and the square shaped combustion chamber.

**Conclusion and perspective**

A consistent flamelet-based framework for turbulent combustion modeling in LRE has been presented using the low-Mach number approximation of the governing equations. All the thermochemical and transport properties have been calculated by means of steady laminar flamelets using a detailed chemical mechanism and transport properties. The proposed framework features the possibility to accommodate, in a computationally efficient manner, real gas thermodynamics and to account for non-adiabatic combustion in the presence of wall heat transfer. These capabilities have been tested on two experimental configurations featuring methane-oxygen flames at elevated pressures, which of technological relevance for LRE applications. Simulations have been carried out using an URANS approach and in both cases, a cryogenic flame and a non-adiabatic single element combustion chamber, the numerical results are in a fairly good agreement with experiments.

Future efforts will be devoted to explore the eddy dissipation concept EDC.
combustion model and to employ the presented framework in realistic multi injectors geometries.

References