Towards an Unsteady/Flamelet Progress Variable method for non-premixed turbulent combustion at supercritical pressures

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Abstract

Combustion devices operating at elevated pressures, such as liquid rocket engines (LRE), are usually characterized by supercritical thermodynamic conditions. Propellants injected into the combustion chamber experience real fluid effects on both their mixing and combustion. Transition through super-criticality implies abrupt variations in thermochemical properties which, together with chemical reactions and high turbulent levels introduce spatial and temporal scales that make these processes impractical to be simulated directly. Reynolds-Averaged Navier-Stokes (RANS) and Large Eddies Simulation (LES) equipped with suitable turbulent combustion modeling are therefore mandatory to attempt numerical simulation on realistic length scales. In the present work, the building blocks for extending the unsteady/flamelet progress variable approach for turbulent combustion modeling to supercritical non-premixed turbulent flames are presented. Such approach requires a large number of unsteady supercritical laminar flamelet solutions at supercritical pressures, usually referred as flame structures, to be preliminarily established by solving the flamelet equations with suitable real fluid thermodynamics. Given such unsteady flame structures, flamelet libraries can then be generated for all thermochemical quantities. The explicit dependence on flamelet time is usually eliminated using mixture fraction, reaction progress parameter, and maximum scalar dissipation rate as independent flamelet parameters. Real fluid thermodynamics used for such unsteady supercritical laminar flamelet solutions, is taken into account by means of a computationally efficient cubic equation of state. In order to have a better handling of real gas mixtures, the real gas equation of state is written in a comprehensive three-parameter fashion. A priori analysis at supercritical pressures of transient flame structures is performed in order to study how solutions populate the flamelet state space which is usually characterized by the S-shape diagram representing a collection of steady solutions. High-pressure conditions ranging from 60 to 300 bar are chosen as representative of a methane/liquid-oxygen rocket engine operating conditions.

1. Introduction

High performance liquid rocket engines (LRE) widely utilize liquid oxygen (LOx) together with liquid hydrogen (LH2) and, more recently liquified natural gas (LNG) as propellants, because of their high specific impulse and non-toxic combustion. Despite the experimental and theoretical effort in the past decades, in-depth understanding of the complex phenomenology taking place in the thrust chamber of a typical LRE, is still to be fully achieved [1].

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Operating conditions of LRE are mainly determined by chamber pressure p_C and injection temperature of the fuel T_f and oxidizer T_{ox}, and are usually classified with respect to the critical properties of the propellants. In most of the practical cases methane is injected in supercritical conditions ($T > T_{cr} = 190.8K$, $p > p_{cr} = 4.599MPa$) while liquid oxygen (LOx) is injected in a transcritical state ($T < T_{cr} = 154.6K$, $p > p_{cr} = 5.043MPa$). The injection temperature of LOx can be significantly lower than the critical temperature of oxygen, typically between $80K$ and $120K$, enhancing real fluid effects on both the mixing and combustion processes, thereby exhibiting sharp gradients of density and abrupt changes of mixture thermodynamical properties. In order to characterize combustion chambers at supercritical pressures [2], unified treatment of fundamental multi-species real gas thermodynamics is mandatory in numerical simulations, as well as detailed chemical kinetic mechanismssuitable for high pressure conditions. Experiments in the past decade [3, 4, 5] have shown that supercritical mixing and combustion can be conceptually based on a single-phase mixture. Thus, numerically, a general fluid is modeled as a "dense" gas with liquid like density and gas like diffusivities that does not experience any droplet formation with a vanishing surface tension.

Turbulence/chemistry interaction models in supercritical reacting flows, both in LES and RANS, are generally based on steady state flamelet assumptions [6, 7]. The aim of the present work, on the other hand, is to establish a framework for the extention to supercritical combustion of unsteady flamelet progress variable (UFPV) approaches [8, 9].

An a priori study of unsteady flamelet solutions, prototypical of transient flame configurations characterized by time dependent features such as re-ignition and quenching, are investigated numerically by means of a general fluid formulation for the unsteady laminar flamelet equations.

2. Supercritical Unsteady Flamelet

In this work, real fluid thermodynamic properties are taken into account by means of a computationally efficient cubic equation of state (EoS) written in a general three-parameter fashion [10] which reads, for a pure species:

$$p = \frac{\rho R_u T}{W - b\rho} - \frac{a\alpha(T)\,\rho^2}{(W + \delta_1 b\rho)\,(W + \delta_2 b\rho)} \tag{1}$$

where p, ρ, T are fluid pressure, density and temperature, W is the molecular weight, R_u the universal gas constant and $\alpha(T)$ is a temperature correction factor. The three parameters characterizing the EoS are a, b and δ_1 (whereas $\delta_2 = (1 - \delta_1)/(1 + \delta_1)$). The choice of parameters in Eq. (1) determines which particular cubic EoS has been chosen. The classical Peng-Robinson form is recovered for $\delta_1 = 1 + \sqrt{2}$ while the Soave-Redlich-Kwong form for $\delta_1 = 1$. A complete three parameter EoS, such as the RK-PR, is obtained for $\delta_1 = \delta_1(Z_c)$, where Z_c is the critical compressibility factor [11], and represents an additional dependence on Z_c. Complete definitions for a, b, α and δ_1 as well as their fitting parameters can be found in work of Cismondi and Mollerup [10].

The validity of the real fluid EoS is extended to an arbitrary number of components, considering a mixture as a single phase and unique pure hypothetical fluid. The parameters required by the EoS are calculated from conventional molar fraction based mixing rules [11] on the basis of the critical state of each pure component, such as critical temperature and pressure as well as acentric factor.

Given the EoS parameters ($a\alpha$,b,δ_1) of a mixture, every thermodynamical relation can be expressed in terms of a reference ideal low-pressure property and a real gas departure function [12] derived from the real gas EoS. In the present case of RK-PR EoS departure functions assume the form derived by Kim et al. [13].
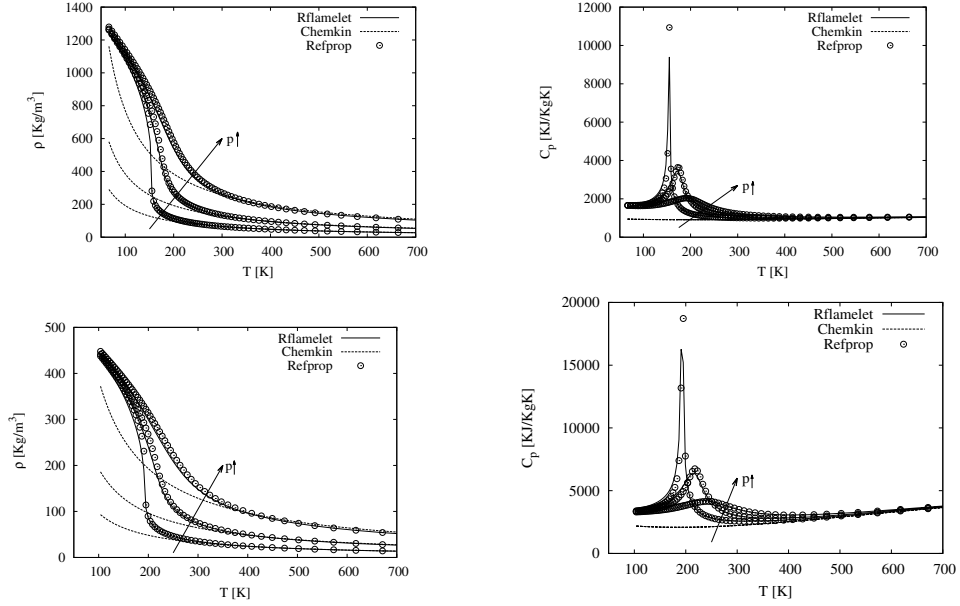
Figure 1: Validation of principal thermodynamic properties: density and constant pressure specific heat of pure oxygen (top) and pure methane (bottom) as a function of temperature at three different pressures, respectively 50bar, 100bar and 200bar. Solid lines (−) are the in-house Rflamelet code results, dashed lines (−−) are Chemkin ideal gas EoS results [14], circles are Refprop software results from the NIST database [15]

In Fig. 1, the thermodynamical properties for both the fuel and the oxidizer, as estimate by the above model, are compared against NIST data. In the proximity of the critical point, thermodynamic and transport properties exhibit anomalies in their behavior, usually referred as near-critical enhancement.

The local flame structure of a turbulent non-premixed flame can be described, in the high Damkohöler limit, by one dimensional flamelet equations in mixture fraction space. Such equations highlight the unsteady competition between chemical kinetics and molecular diffusion processes enhanced by turbulent mixing. The diffusion parameter of the flamelet equations is the scalar dissipation rate χ of the mixture fraction z defined as $\chi = 2D(\nabla z)^2$, where D is the diffusion coefficient of z. Assuming unitary Lewis-number and using the energy equation in terms of enthalpy derivatives in order to avoid numerical issues due to constant pressure specific heat, c_p, enhancement, flamelet equations read [16]:

$$\frac{\partial Y_i}{\partial t} = \frac{1}{2}\chi\frac{\partial^2 Y_i}{\partial z^2} + \frac{\dot{\omega}_i}{\rho} \quad ; \qquad \frac{\partial T}{\partial t} = \frac{1}{2}\chi\frac{1}{c_p}\Big[\frac{\partial^2 h}{\partial z^2} + \sum_{k=1}^{ns} h_k\frac{\partial^2 Y_k}{\partial z^2}\Big] + \frac{\dot{\omega}_T}{c_p\rho} \qquad (2)$$

The solution of the flamelet system, equations (2), defines the flame structure in mixture fraction z-space. The functional dependence of the scalar dissipation rate on mixture fraction can be assumed as that stemming from a temporal mixing layer in physical space and reads $\chi(z,t) = \chi_{max}(t)\exp(-2\text{erfc}^{-1}(2z))^2$.

We solve the time dependent flame structure in a fully coupled fashion, thus no operator splitting technique was adopted, the whole system being integrated using a stiff solver for ordinary differential equations. This unsteady flamelet system has been recently used to analyze supercritical methane/LOx auto-igniting flame structures [17].

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3. Results and Discussion

As previously mentioned, state-of-art supercritical combustion CFD simulations currently rely on simplified steady state flamelet models where chemistry is assumed to respond infinitely fast to perturbations from the turbulent flow field. In a high pressure environment the reduces kinematic viscosity and thus elevated Reynolds number, can lead to rapid and intense scalar dissipation rate variation, due to its intermittent nature [18]. Therefore a turbulent combustion model, such as the UFPV method, that can represent unsteadiness in the flame structure arising from scalar dissipation rate fluctuations can become crucial [8, 9].

The response of laminar, methane/LOx, supercritical flamelets to turbulent perturbations is investigated in a a priori fashion by means of representative synthetic signals. Turbulent effects are modeled as abrupt changes or sharp signals in time of the scalar dissipation rate [19]. Following [20] the scalar dissipation rate profile fluctuates with a factor $\phi(t)$ that can vary from 0.5 to 2:

$$\chi(z, t) = \phi(t)\chi_{max} \exp(-2 \mathrm{erfc}^{-1}(2z))^2 \tag{3}$$

In the above scalar dissipation rate signal, $\phi(t)$ is chosen as a triangular wave [19]. This signal is completely characterized by a peak amplitude A_χ and a duration τ_χ as shown in Fig. 2. The signal $\phi(t)$ is imposed to the supercritical flamelet system, starting from a steady state solution found for a scalar dissipation rate near the quenching value.

Realistic LOx-Methane LRE combustion chamber conditions for supercritical flamelet calculations are employed, with a background pressure of 60 bar. Flamelet boundary conditions are pure oxygen at the oxidizer side (T_{ox} = 120 K) and pure methane at the fuel side (T_{fuel} = 300 K). A detailed chemical kinetic mechanism for methane oxidation at elevated pressures, referred to as Ramec [21], is used throughout this study. The scalar dissipation rate model is expressed as in eq. (3), and the initial condition is a steady state flamelet solution obtained for $\chi_{max} = 50000s^{-1}$.

For a given perturbation time τ_χ it is possible to find a critical perturbation amplitude $A_{\chi_{cr}}$ which marks the bifurcation between quenching and re-ignition of a steady state burning flame structure. The characteristic time τ_χ has been chosen of the order of a Kolmogorov timescale τ_K on the basis of experimental and numerical data for hydrogen/LOx combustion at elevated pressure [22], in which such a timescale was estimated at $\tau_K \approx 1 \mu$s. For the near critical pressure of 60 bar, the critical perturbation amplitude is found to be $A_{\chi_{cr}}$ = 1.329. The bifurcational behavior of the flame structure subject to scalar dissipation rate signals around the critical perturbation amplitude, is shown in terms of heat release rate (HRR) and peak temperature in time Fig. 2.
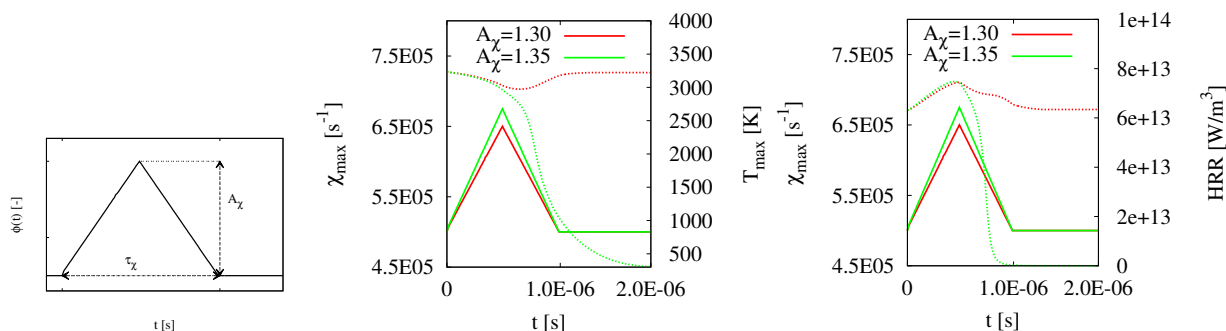

Figure 2: Scalar dissipation rate signal (left), characterized by function $\phi(t)$, a triangular wave defined by an amplitude A_χ and a duration τ_χ. Time evolution of peak temperature (middle) and heat release rate (right) during signals around the critical amplitude.

The signal characterized by $A_\chi = 1.30$ will allow the re-ignition of the flame structure with the flamelet peak temperature promptly recovering the initial steady state value. On the other hand the signal characterized by $A_\chi = 1.35$, because of the increased heat losses will cause the ultimate quenching of the flame structure with rapid decrease of the peak flamelet temperature toward the mixing lines values. Similar observations can be made for the heat release rate, with the only difference that during the first part of the signal when the scalar dissipation rate is increasing, HRR is also increasing since it is still diffusion controlled.
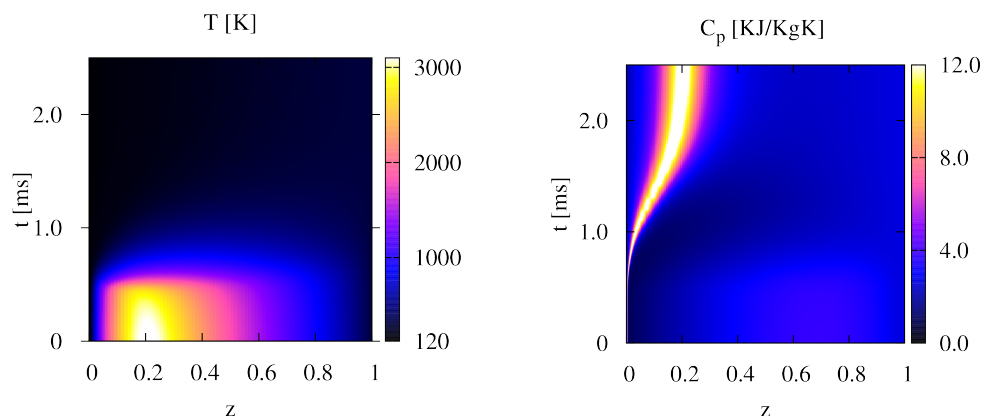

Figure 3: Real gas flame structure results for a scalar dissipation rate signal characterized by $A_\chi = 1.35$ and $\tau_\chi = 1\,\mu s$ leading to quenching: Temperature $T(z,t)$ (left) and constant pressure specific heat of the mixture $C_p^{mix}(z,t)$ (right)

Figure 3 exhibits the unsteady quenching solution signature in (z,t) space. In particular $T(z,t)$ is seen to abruptly relax towards the quenched, adiabatic mixing line solution. The $c_p(z,t)$ solution, on the other hand, gradually recovers a clear peak due to near-critical enhancement, which moves to richer values of mixture fraction. In the steady ignited solution, such a peak was confined far nearer the LOx side, permanently acting as a a heat sink [17] for the energy equation (2), thus enhancing the quenching phenomena.
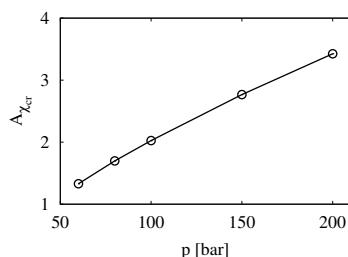

Figure 4: Critical amplitude of the scalar dissipation rate triangular signal $A_{\chi_{cr}}$ at various supercritical pressures.

Figure 4 shows how pressure influences the crital amplitude $A_{\chi_{cr}}$ for a given perturbation time. In a similar manner to the quenching value of the scalar dissipation, $A_{\chi_{cr}}$ is obseved to increase almost linearly with pressure. While this hints at a greater absolute resilience of high pressure flames to scalar dissipation perturbations - essentially due to a greater heat release rate - it is equally true that at high pressures, enhanced kinetic timescales are expected to reduce the extent to which scalar dissipation can be increased relative to the quenching value, for the same perturbation time τ_χ.

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4. Conclusion and perspective

An a priori analysis of transient LOx-Methane flame structures has been carried out at supercritical pressures, utilizing an unsteady laminar flamelet model as a building block of an UFPV method. High-pressure conditions have been chosen as representative of a LOx-Methane rocket engine operating conditions. Real gas effects have been taken into account in unsteady multi-component reacting calculations by means of a comprehensive three parameter equation of state. Re-ignition and quenching of the flame structure under synthetic turbulent perturbations has been studied using scalar dissipation rate signals. A critical scalar dissipation amplitude has been observed to increase with pressure. Transient flamelet solutions are expected to populate the flamelet state space plane and can thus be representative of flamelet libraries for an unsteady flamelet progress variable approach. From the combustion modeling point of view additional effort is still needed in order to take into account radiative heat losses, differential diffusion and soot formation.

References

[1] G.P. Sutton and O. Biblarz. *Rocket Propulsion Elements*. John Wiley and Sons, New Jersey, 8th Edition, 2010.

[2] V. Yang. Modeling of supercritical vaporization, mixing, and combustion processes in liquid-fueled propulsion systems. *Proceedings of the Combustion Institute*, 28(1):925–942, 2000.

[3] P. Scouflaire, J-C. Rolon, S. Candel, M. Juniper, and a. Tripathi. Structure of cryogenic flames at elevated pressures. *Proceedings of the Combustion Institute*, 28(1):1103–1109, 2000.

[4] G. Singla, P. Scouflaire, C. Rolon, and S. Candel. Transcritical oxygen/transcritical or supercritical methane combustion. *Proceedings of the Combustion Institute*, 30(2):2921–2928, January 2005.

[5] M. Habiballah, M. Orain, F. Grisch, L. Vingert, and P. Gicquel. Experimental Studies of High-Pressure Cryogenic Flames on the Mascotte Facility. *Combustion Science and Technology*, 178(1-3):101–128, January 2006.

[6] S. Candel, T. Schmitt, M. Boileau, and Y. Méry. Large-Eddy Simulation of oxygen/methane flames under transcritical conditions. *Proceedings of the Combustion Institute*, 33(1):1383–1390, 2011.

[7] T. Kim, Y. Kim, and S.K. Kim. Real-fluid flamelet modeling for gaseous hydrogen/cryogenic liquid oxygen jet flames at supercritical pressure. *The Journal of Supercritical Fluids*, 58(2):254–262, September 2011.

[8] H. Pitsch and M. Ihme. An unsteady/flamelet progress variable method for les of nonpremixed turbulent combustion. *AIAA Journal, 2005-557*, 2005.

[9] M. Ihme and Yee Chee See. Prediction of autoignition in a lifted methane/air flame using an unsteady flamelet/progress variable model. *Combustion and Flame, 157 18501862*, 2010.

[10] M. Cismondi and J. Mollerup. Development and application of a three-parameter RKPR equation of state. *Fluid Phase Equilibria*, 232(1-2):74–89, 2005.

[11] R.C. Reid, J.M Prausnitz, and B.E. Poling. *The properties of Gases and Liquids*. McGraw-Hill, New York, NY, 2001.

[12] Richard S Miller and Josette Bellan. Efficient High-pressure State Equations. *AIChE Journal*, 43(6):4–9, 1997.

[13] S.K. Kim, H.S. Choi, and Y. Kim. Thermodynamic modeling based on a generalized cubic equation of state for kerosene/LOx rocket combustion. *Combustion and Flame*, 159(3):1351–1365, March 2012.

[14] R.J. Kee, F.M. Rupley, and J.A. Miller. *Chemkin II: A FORTRAN package for analysys of gas phase chemical kinetics*. Sandia National Laboratories, 1993.

[15] Refprop. *http://webbook.nist.gov/chemistry/fluid*. National Institute of Standards and Technology Webbook, 2014.

[16] T. Kim, Y. Kim, and S.K. Kim. Numerical analysis of gaseous hydrogen/liquid oxygen flamelet at supercritical pressures. *International Journal of Hydrogen Energy*, 36(10):6303–6316, May 2011.

[17] P. E. Lapenna, P. P. Ciottoli, M. Valorani, and F. Creta. Numerical investigation of unsteady laminar methane/lox flamelet at supercritical pressures. European Combustion Meeting 2015, Budapest, Hungary.

[18] Stephen B Pope. *Turbulent flows*. Cambridge university press, 2000.

[19] John C. Hewson. An extinction criterion for nonpremixed flames subject to brief periods of high dissipation rates. *Combustion and Flame*, 160(5):887 – 897, 2013.

[20] Y. Xuan and G. Blanquart. A flamelet-based a priori analysis on the chemistry tabulation of polycyclic aromatic hydrocarbons in non-premixed flames. *Combustion and Flame*, 161(6):1516 – 1525, 2014.

[21] E.L. Petersen, D.F. Davidson, and R.K. Hanson. Kinetics Modeling of Shock-Induced Ignition in Low-Dilution CH 4 / O 2 Mixtures at High Pressures and Intermediate Temperatures. 290:272–290, 1999.

[22] B Ivancic and W Mayer. Time-and length scales of combustion in liquid rocket thrust chambers. *Journal of propulsion and power*, 18(2):247–253, 2002.