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# The impacts of three flamelet burning regimes in nonlinear combustion dynamics

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ABSTRACT

Axisymmetric simulations of a liquid rocket engine are performed using a delayed detached-eddy-simulation (DDES) turbulence model with the Compressible Flamelet Progress Variable (CFPV) combustion model. Three different pressure instability domains are simulated: completely unstable, semi-stable, and fully stable. The different instability domains are found by varying the combustion chamber and oxidizer post length. Laminar flamelet solutions with a detailed chemical mechanism are examined. The $\beta$ probability density function (PDF) for the mixture fraction and Dirac $\delta$ PDF for both the pressure and the progress variable are used. A coupling mechanism between the volumetric Heat Release Rate (HRR) and the pressure in an unstable cycle is demonstrated. Local extinction and reignition are investigated for all the instability domains using the full S-curve approach. A monotonic decrease in the amount of local extinctions and reignitions occurs when pressure oscillation amplitude becomes smaller. The flame index is used to distinguish between the premixed and non-premixed burning mode in different stability domains. An additional simulation of the unstable pressure oscillation case using only the stable flamelet burning branch of the S-curve is performed. Better agreement with experiments in terms of pressure oscillation amplitude is found when the full S-curve is used.



## 1. Introduction

In recent years, there is an increasing need for computational efficient numerical tools to simulate accurately the combustion dynamics in high-power propulsion engines such as liquid rocket engines, scramjets, and gas turbine engines. A popular method is the finite-rate chemistry model where filtered/Favre-averaged species transport equations are solved. Different approaches have been taken to address the closure problem that arises from the filtered reaction source terms. In the Laminar Closure Model (LCM), the Arrhenius reaction law is applied directly using the mean quantities [1,2]. In the Eddy Dissipation Model [3], the reaction source terms are calculated based on turbulence quantities and different constants. In the Thickened Flame Model approach, flames are artificially thickened to be resolved on numerical grids by multiplying the diffusion and dividing the reaction rates by a thickening factor [4,5]. Another approach is the Linear Eddy Mixing (LEM) model [6,7], in which the relevant advection–diffusion–reaction couplings are resolved using a low-dimensional representation of turbulent advection. Therefore, in these models, incorporating any realistic detailed-chemical mechanism involving tens of species and hundreds of reactions presents a difficult challenge due to the enormous computational cost. Additionally, the nonlinearity of species reaction source terms and the wide range of chemical time scales associated with these schemes make the resulting species transport equations very stiff and difficult to solve. Therefore, most of these models are limited to either one- or two-step chemical mechanisms involving four-five species. The transported probability density function (PDF) [8,9] is arguably the best closure model for chemistry–turbulence interaction, as it does not require any additional model for the chemical source terms. However, because of the high dimensionality of its argument, the model requires Monte-Carlo simulations of at least 30–50 notional particles in a cell. The PDF simulations are, thus, usually very computationally expensive even with a simple chemistry model [8].

An alternative model to the above method is the flamelet approach. In the flamelet concept, the chemical time scales are shorter than the turbulent time scales so that the flame can be viewed as a collection of laminar flamelets [10]. This definition allows the chemistry computation to be performed independently of the main flow simulation and pre-process as flamelet libraries/tables. Therefore, complex chemical mechanisms can be used without incurring additional computational cost on the main flow calculations. The flamelet approach has been applied

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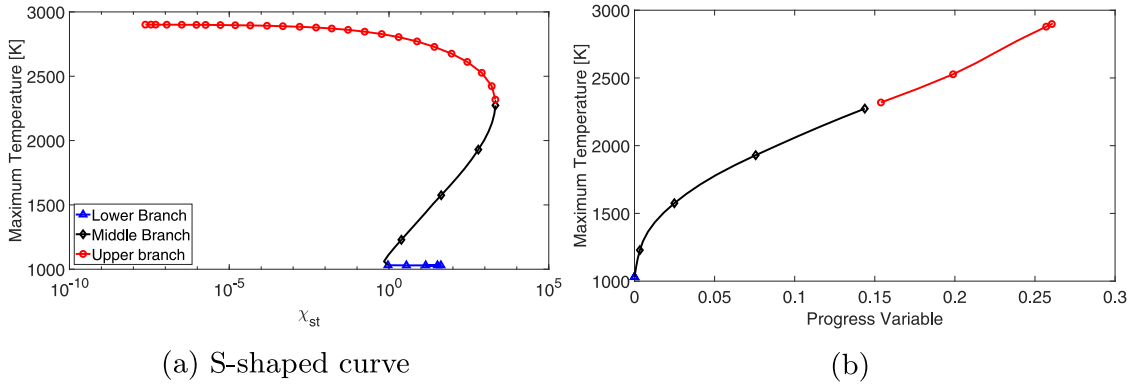


**Fig. 1.** Solutions of the steady flamelet equations for methane/oxygen combustion with $T_f = 300$ K and $T_o = 1030$ K.

successfully to turbulent premixed flames [11–14] as well as non-premixed flames [15,16]. In the steady laminar non-premixed flamelet approach, the thermo-chemical quantities are solved in the mixture fraction space using

$$-\frac{\rho\chi}{2}\frac{\partial^2\psi_i}{\partial Z^2} = \dot{\omega}_i \tag{1}$$

where $\psi_i$ can be any reactive scalar quantities such as species mass fractions and temperature. The solutions of these equations can be represented by an S-curve, as shown in Fig. 1a.

Figure 1a shows the maximum flame temperature as a function of the stoichiometric scalar dissipation rate $\chi_{st}$. This S-shaped curve illustrates the nature of diffusion flamelets. Each scalar dissipation rate could have multiple solutions; it is thus not a well-defined function (Fig. 1a).The upper branch describes stable burning solutions (curve with circle markers). The lower branch (horizontal line with triangle markers) describes non-burning solutions. The middle branch (line with diamond markers) shows the unstable burning solutions. The traditional diffusion flamelets approach of Peters [10] can only cover the upper branch. The Flamelet Progress Variable (FPV) approach, first introduced by Pierce and Moin [17], can cover all 3 branches because all the relevant quantities (e.g. maximum temperature) become monotonic functions of the progress variable (C) (Fig. 1b). Simulating a coaxial jet combustor, similar to the configuration used in this work, Pierce and Moin compared the FPV model to a fast-chemistry model and a traditional non-premixed steady-flamelets approach. The FPV approach predicted the correct flame liftoff behavior compared with the steady flamelet approach while agreeing well with the experimental time-averaged velocities and temperature. Since the seminal work of Pierce and Moin, many researchers have successfully applied and extended the baseline FPV to various non-premixed and partially premixed flames. Ihme et al. [18,19] studied local extinction and reignition effects in non-premixed turbulent combustion using the FPV model. The authors first compared the traditional presumed PDF ($\beta$ PDF for the mixture fraction and Dirac $\delta$ for the progress variable) with different Statistically Most Likely Distribution (SMLD) PDFs. The extended FPV model is then applied to simulations of the Sandia flames D and E. Improvements in predicting local flame extinctions and reignitions compared to the baseline FPV model were found. However, prior knowledge of the SMLD PDFs is required, making it a less appealing approach compared to the baseline FPV model. Knudsen and Pitsch [20] proposed a multi-regime models by using a modified progress variable source term to distinguish between the premixed and non-premixed combustion regimes.

The works described above primarily simulate flames in the incompressible limit. In the compressible limit, the neglect of the transient pressure effect in the flamelet formulation poses a theoretical inconsistency. However, in this work, both the time and length scales of the pressure oscillation in the chamber are much larger than those of the flamelets. Thus, a quasi-steady pressure assumption, in which the $\partial P/\partial t$ in the flamelet formulation, at any point during the pressure oscillation cycle can be justified. Moreover, the model presented below has even been applied successfully to supersonic and hypersonic combustion [21–23]. The model from here on will be called Compressible Flamelet Progress Variable (CFPV). Pecnik et al. [21] simulated supersonic combustions in the Hyshot II Scramjet engine using Reynolds-Averaged-Navier-Stokes (RANS) turbulence model with the CFPV combustion model. Saghafian et al. [22,23] simulated combustion of a jet in a supersonic cross flow and the HiFiRE Scramjet engine using large-eddy-simulation (LES) with the same CFPV model.

There is no combustion instability observed in any of these simulations. Additionally, to the best of the authors' knowledge, the CFPV model has not been applied to study subsonic compressible combustion. Therefore, this work examines the CPFV model capability in simulating combustion instability in a single-injector rocket engine called Continuously Variable Resonance Chamber (CVRC) [24–27]. Figure 2 shows a simplified schematic of the CVRC computational domain.

Different stability domains were found in the CVRC experiments by varying the oxidizer post lengths from 9 cm to 19 cm. Existing computational results using various turbulence and combustion models for these experiments are available [1,6,28,29]. Srinivasan et al. [6] studied flame dynamics of different stability domains using LES turbulence model coupled with the LEM combustion model. Garby et al. [28] studied both axisymmetric and fully 3D flame stabilization mechanism for the 12-cm oxidizer post using LES method coupled with the Dynamic Flame Thickened chemistry model. Harvazinski et al. [1] studied the effects of grid resolution and dimensionality on the ability to predict combustion instability using both axisymmetric and 3D Detached Eddy Simulations (DES) with the LCM combustion model. Results from these simulations indicate that, while axisymmetric calculations capture the correct wave dynamics, they under-predicted the pressure oscillation amplitudes compared to three-dimensional simulations and experimental results. These simulations used either one- or two-step global chemical mechanisms. Sardeshmukh et al. [30] significantly improved oscillation amplitude predictions for their axisymmetric calculations by using the LCM combustion model with the GRI-Mech 1.2 detailed mechanism. However, 32 species transport equations were solved, making the computational cost prohibitively expensive.

Nguyen et al. [31] recently developed a computationally inexpensive axisymmetric solver utilizing the CFPV and Delay Detached Eddy Simulation (DDES) models. The code is a multi-block finite difference solver. Advection and diffusion terms are discretized

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