



Capabilities and limitations of multi-regime flamelet combustion models

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ABSTRACT

Flamelet combustion models typically assume that burning occurs in either a fully premixed or a fully non-premixed mode. These assumptions tend to limit the applicability of the models to single-regime combustors. Efforts aimed at reducing this limitation have introduced multi-regime approaches that account for different types of mixing and chemistry interactions. In this study a multi-regime model is applied to two laminar *n*-heptane flames in an effort to characterize the capabilities and limitations of the approach. Both a 2-D laminar triple flame and a 2-D laminar counter-flow diffusion flame are numerically simulated using the multi-regime model. Data for comparison is generated by additionally simulating the flames using finite rate chemistry, a purely premixed flamelet model, and a purely non-premixed flamelet model. Simulations demonstrate that the multi-regime approach functions as desired, and tends to access flamelets from the appropriate regime under both non-premixed and premixed conditions. Some important differences between the flamelet solutions and finite rate solution are observed, however. These differences are caused by the finite rate solution deviating away from the assumed flamelet manifolds, rather than by inadequate regime predictions. In the analyses of these simulations, an emphasis is placed on understanding the formation of the pollutant species NO. It is shown that even when the local combustion regime is correctly predicted, small deviations from an assumed flamelet manifold can lead to changes in the NO production rate. The simulation results confirm that multi-regime flamelet models are applicable to a wide variety of reacting flows, but the results also help to characterize the limitations of these models.

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1. Motivation and objective

Flamelet-type turbulent combustion models [1–8] make particularly strict assumptions about how mixing processes and chemistry interact. For example, flamelet models that rely on the non-premixed flamelet equations [9–11] are strictly valid only in the non-premixed combustion regime where fuel and oxidizer enter reaction zones from opposing directions. Similarly, flamelet models that rely on the premixed flamelet equations [12–14] are strictly valid only in premixed combustion regimes where fuel and oxidizer enter reaction zones in a fully mixed state. In many reactive flows, the assumption of a single burning regime is valid and a traditional flamelet implementation describes combustion accurately [2,9,10,12]. In other flows, however, combustion occurs in multiple or mixed regimes in which single regime assumptions no longer hold. For example, modern gas turbine designs often consist of a series of lean premixed burners operating in conjunction with a non-premixed pilot burner. Similarly, recent simulations [15–17] that mimic spray fueled aircraft combustors have been shown to exhibit significant amounts of both premixed and non-premixed

combustion. If these flows are to be described in a flamelet context, traditional models must be extended beyond single regime implementations.

Multi-regime flamelet modeling has been the subject of several research efforts. These efforts generally address three modeling needs: (1) a method of distinguishing between combustion regimes, (2) a method of treating each individual regime, and (3) a method of describing regime interactions. The first of these three components represents the major part of the multi-regime modeling challenge, and several regime indicators that deal with this challenge can be considered. The most traditional approach for distinguishing between regimes is the flame index [18–20], which is constructed by examining whether gradients of fuel and oxidizer align. Modified versions of this index that extend its applicability have also been formulated [5]. A more recent regime indicator has been derived using flamelet transformations and operates by considering the relative magnitude of a series of Damköhler numbers describing different physical processes [6]. While this second indicator allows unsteady combustion processes to be considered, its developers also proposed a more straightforward multi-regime model that directly used the progress variable to distinguish between auto-ignition and premixed combustion [6]. A third multi-regime modeling approach [21] is to form a regime indicator implicitly by solving flamelets in

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a 2-D mixture fraction and progress variable space. The relative magnitude of the scalar dissipation rates in this space serves as an implicit description of the regime. Finally, a fourth approach to regime selection has been derived [7] using a flamelet type transformation that accounts for the statistical dependence of the mixture fraction variable and the progress variable. In this last indicator, the budget of the transformed equation is used to locally determine the importance of each combustion regime.

Once a method of distinguishing between regimes is selected, a number of traditional flamelet models [2,4,12,13,22] could be employed to describe the combustion occurring within each distinct regime. Similarly, a number of methods that attempt to model how transitions occur between these regimes can be envisioned or formulated. These methods range from the computationally inexpensive approach of blending 1-D flamelet solutions from different regimes [5,7,19] to the more expensive approach of allowing for the interaction of different regimes in flamelet space [21].

While approaches to multi-regime modeling are now available, a variety of questions regarding their accuracy and validity remain open. For example, existing validation studies of multi-regime approaches have been performed using steady 1-D domains [5] and in flamelet space [21]. These studies, however, do not completely represent higher dimensional settings in which diffusion can occur along multiple vectors that are arbitrarily aligned. A select number of Large Eddy Simulation (LES) multi-regime studies also exist [7,19], but the complexity and filtering operations associated with these studies often preclude the full analysis of where errors may be introduced by multi-regime approaches. Finally, while data from direct numerical simulations of highly turbulent flows should be used to test the assumptions in all models, the examination of less complex flame data in which the most significant effects of turbulence and chemistry interaction are separated allows for a more complete analysis of any underlying multi-regime combustion modeling assumptions.

The objective of this study is to use computations of two laminar flames to assess both the capabilities and the shortcomings of a multi-regime flamelet approach. Two particular questions motivate the study. First, how well can mixed regime flames be described using flamelets from discrete regimes? Second, can the leading order inaccuracies in the modeled flame be traced to an incorrect description of the regime, or are these inaccuracies due to other factors? These questions will be answered by using finite rate chemistry to simulate the flames under consideration, and then using flamelet approaches to model this ‘true’ finite rate solution. Using this data, it will be shown that the multi-regime approach functions very accurately and captures the appropriate combustion mode in each of the flames that are considered. The accuracy of the multi-regime approach will be emphasized by demonstrating that the observed differences between the finite rate solution and the flamelet solutions are due to the finite rate solution deviating from flamelet manifolds, rather than to an incorrect blend of regimes.

This introduction represents Section 1 of the paper. The single and multi-regime flamelet implementations that are used as baseline models are reviewed in Section 2. The laminar flame configurations are then introduced in Section 3. The results of a triple flame simulation are presented in Section 4, while the results of a counterflow simulation are presented in Section 5. A brief concluding summary is provided in Section 6.

2. Combustion modeling approaches

2.1. Chemistry and flow solver

The flames in this study are simulated using both a typical finite rate chemistry approach and several flamelet modeling approaches.

A reduced *n*-heptane mechanism [23] is used to describe chemical kinetics in all of the combustion calculations that are performed. This reduced mechanism consists of 44 species, 24 of which are algebraically solved by employing steady state assumptions. The *n*-heptane mechanism does not include any nitrogen chemistry, and in order to consider the formation of NO two species and two reactions are added to the original 44 species mechanism. The two added reactions are



where N_2 , O_2 , and O are present in the original mechanism but where the NO and N species have been added. The rates for the two added reactions are taken directly from the GRI 3.0 mechanism [24].

Different Lewis number assumptions might be made within any self-contained model validation framework. For example, in laminar flames non-unity Lewis numbers would be appropriate. Additionally, the non-unity Lewis number assumption would be needed for turbulent premixed combustion modeling. In the context of turbulent non-premixed combustion modeling, however, a unity Lewis number assumption might be more appropriate [25,26]. In the simulations that follow the goal is to isolate the importance of regimes in the absence of modeling challenges such as radiation or differential diffusion effects. Unity Lewis numbers are therefore used in both the physical space and flamelet space calculations that will be presented. The diffusivity of all scalars, including the mixture fraction scalar that is defined below, is set equal to the diffusivity of the gas enthalpy. This enthalpy diffusivity changes as the local gas composition and temperature change. The molecular viscosity also changes with the gas composition. Consequently, Schmidt numbers vary throughout the flow, but are the same for all species at any given location.

The flow solver that is used for the flame simulations is a structured finite-difference code [27] that solves the Navier–Stokes and scalar transport equations in the low Mach number limit,

$$\frac{\partial}{\partial t}(\rho) + \frac{\partial}{\partial x_j}(\rho u_j) = 0, \quad (3)$$

$$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}(\rho u_i u_j) = -\frac{\partial}{\partial x_i}(p) + \frac{\partial}{\partial x_j}(\sigma_{ij}), \quad (4)$$

$$\frac{\partial}{\partial t}(\rho \phi_k) + \frac{\partial}{\partial x_j}(\rho u_j \phi_k) = \frac{\partial}{\partial x_j}(\rho \phi_k V_{kj}^{diff}) + \rho \dot{\omega}_k, \quad (5)$$

$$\begin{aligned} \frac{\partial}{\partial t}(\rho T) + \frac{\partial}{\partial x_j}(\rho u_j T) = & \frac{1}{c_p} \left[\frac{\partial}{\partial x_j} \left(\rho \mathcal{D}_T \bar{c}_p \frac{\partial T}{\partial x_j} \right) + \rho \dot{Q} \right] \\ & + \frac{1}{c_p} \left[\sum_k \left(\rho c_{p,k} \frac{\partial T}{\partial x_j} \phi_k V_{kj}^{diff} \right) \right], \end{aligned} \quad (6)$$

where

$$\phi_k V_{kj}^{diff} = \mathcal{D}_k \frac{\partial \phi_k}{\partial x_j} + \mathcal{D}_k \frac{\phi_k}{W} \frac{\partial \bar{W}}{\partial x_j} + \phi_k V_{kj}^{corr}. \quad (7)$$

In these equations ρ is the density, u_i is the velocity in the i th direction, and ϕ_k is a scalar representing a species mass fraction. T is the temperature, p is the pressure that is used to enforce continuity, σ_{ij} is the viscous stress tensor, and W is the molecular weight. The diffusion velocity of species k in the j th direction is V_{kj}^{diff} , and the correction velocity that appears in this term, V_{kj}^{corr} , is computed so that the diffusive flux of mole fractions sums to zero [28,29]. $\dot{\omega}_k$ is the chemical source term for species k and \dot{Q} is the heat release. Overbars in these expressions denote mixture averaged quantities, and $c_{p,k}$ is the specific heat of species k . The code is run using implicit

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