Combustion and Flame 161 (2014) 1735–1743

Contents lists available at ScienceDirect

Combustion and Flame

journal homepage: www.elsevier.com/locate/combustflame

Natural parameterizations of flame structure and heat release in lean premixed CH_4/air combustion

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ARTICLE INFO

Article history:
Received 31 August 2013
Received in revised form 10 November 2013
Accepted 20 December 2013
Available online 11 January 2014

Keywords:
Premixed flames
Laminar flames
Detailed chemistry
Self-similarity
Reaction pathways

ABSTRACT

In reduced-order modeling of premixed combustion, a major concern is whether chemistry submodels capture flame characteristics over a broad range of mixture stoichiometries and reactant temperatures. In order to adapt to local temperature level and stoichiometry, models require a suitable parameterization. Post-processing of a large database of adiabatic laminar flame simulations reveals that characteristic temperatures within premixed flames can be collapsed to self-similar structures throughout the lean and ultra-lean premixed regime. The collapse depends on the parameterization, where adiabatic flame temperatures T_{ad} and stoichiometry Φ are identified as natural primary and secondary parameters, respectively. Furthermore, parameterizations of chemical source terms are superior to parameterizations of species profiles, as they allow for a differentiation of chemical processes from transport processes. A comparison of flame characteristics at low and high T_{ad} illustrates that reaction pathways and resulting contributions to the heat release by individual reactions shift according to the temperature level, whereas flames with comparable T_{ad} have similar flame structures that are almost independent of initial temperatures and stoichiometries.

1. Introduction

The development of advanced lean and ultra-lean combustion systems relies heavily on accurate numerical tools and chemistry submodels [1]. Enormous progress has been made in the understanding of chemical kinetics; the resulting detailed mechanisms are, however, impractical for large-scale combustion simulations, as even relatively simple configurations result in exorbitant computation times. An intuitive approach replaces detailed kinetics by reduced models.

The present state of reduced order chemistry modeling can be categorized by two distinct philosophies: (1) mechanism reduction and (2) flamelet models with tabulated chemistry. In technical terms, the two approaches can be distinguished based on the extent of the domain used for the description of thermo-chemical processes. Mechanism reduction focuses on locally defined states and rate expressions, where various automated model reduction approaches use the Jacobian of chemical source terms for a detailed investigation, e.g. ILDM [2,3], CSP [4], and CEMA [5,6]. On the other hand, flamelet models and closely related flamelet-generated manifolds take a global approach, where entire solutions are tabulated either in physical space or composition space [7–11]. Both approaches have their advantages and disadvantages: while approach (1) gives accurate results, simplified mechanisms are still large. Approach (2) allows for efficient simulations with a small number of parameters, but parameterizations are largely ad hoc. Common parameter choices include input parameters (e.g. unburned mixture temperature, stoichiometry, and pressure) and locally evaluated quantities (e.g. progress variables based on local temperature or major species, strain rate, atomic mass fractions). Flamelet formulations fail for ignition phenomena before a flame is established, or when reactions freeze prior to complete combustion, e.g. in IC engines. In both cases, it is difficult to relate actual physical processes to data that are tabulated for a different combustion regime.

A major goal of this study is to systematically identify *natural* parameterizations for generic flame structures. In the following, different terms are used to differentiate between *attributes* that are defined at a global level, and *characteristics* that describe progressions within the flame structure. E.g., the laminar burning flux $\dot{m}_L$ constitutes an attribute as it describes the entire flame, whereas the temperature where an intermediate species peaks would correspond to a characteristic. As characteristics are defined on progressions that have a unique definition throughout the flame structure, they are distinct from *indices* derived from local Jacobians, – e.g. explosive indices and participation indices in the context of CEMA, – which are based on local eigenvalues and eigenvectors and thus do not have a unique interpretation.

Using characteristics that gauge the effect of reaction chemistry, it is possible to investigate how reaction pathways in a flame struc-

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http://dx.doi.org/10.1016/j.combustflame.2013.12.021

ture change according to the operating conditions. A critical aspect of a natural, universally applicable, parameterization of flame characteristics is that it is not necessarily limited to conventional regimes that are typically associated with atmospheric conditions, i.e. standard temperature and pressure (STP). In order to emulate the impact of preheating on combustion of CH_4/air mixtures with arbitrary stoichiometry, a data base with pseudo-randomly distributed initial conditions is created. Using an a posteriori, data-driven approach, the goal is to identify shared patterns within flame structures of freely propagating, adiabatic flames, and to derive a suitable parameterization that reflects underlying physical processes. The current work builds on a precursor study on rich CH_4/air flames, where it was shown that the transition from the preheating zone to an active reaction layer correlates with the laminar burning flux $\dot{m}_L$ [12]. In the following, a more general parameterization of flame characteristics is introduced in order to capture the entire flame structure of lean CH_4/air combustion over a broad range of conditions.

2. Numerical approach

2.1. Numerical method

Simulations are based on standard governing equations for laminar flame propagation with detailed reaction kinetics [13]. All numerical data presented in the current study were obtained using Cantera 2.0.2 [14] and the detailed San Diego chemical kinetics mechanism [15] with 46 species and 235 reactions. In all cases, adiabatic flame simulations were run with non-uniform grid spacing. After obtaining an initial result, the domain length was adjusted to $[-10\,\delta_L^0, 40\,\delta_L^0]$, with δ_L^0 representing the flame thickness based on the temperature gradient. Also, the time step was adjusted to $5\times10^{-7}/\dot{m}_L$, where $\dot{m}_L$ is the laminar burning flux; relative and absolute tolerances for cantera's solver were set to 10^{-12} and 10^{-15}, respectively. Tight grid spacing was assigned to zones with large temperature gradients by projecting 360 equi-spaced values of the monotonically increasing function $z/50\delta_L^0 + 3T(z)/\Delta T_{ad}$ back onto the axial coordinate z, where T is the gas temperature and ΔT_{ad} is the adiabatic temperature increase.

2.2. Database

For laminar CH_4/air flames, initial conditions are uniquely defined by the initial temperature T_{in} and the mixture stoichiometry, which is specified by the normalized equivalence ratio $\Phi \equiv \phi/(\phi+1)$ [16]. Inlet conditions follow a pseudo-random Sobol sequence [17] on the (T_{in}/Φ) plane, where extents for T_{in} (300–1000 K) and Φ (0.1–0.5) were selected. Pseudo-random sequences systematically add sample points with an almost uniform increase in sample point density. Among 1024 sample points, 628 cases are considered viable with converged solutions and non-marginal flame behavior.

The two most fundamental results of laminar flame speed simulations are adiabatic temperature T_{ad} and laminar burning flux $\dot{m}_L$ with units [kg/m^2 s]. While the former concept is straight-forward, the latter definition is chosen to unambiguously define the feed rate of reactants based on a conserved scalar. In order to eliminate cases with marginal flammability, only cases with $\dot{m}_L > 0.05$ kg/m^2 s and $T_{ad} > 1420$ K are considered.

Figure 1 illustrates the data base with 1024 inlet conditions and 628 viable results. The data are illustrated both in terms of (T_{in}/Φ) and (T_{in}/ϕ); using the normalized equivalence ratio Φ rather than the conventional equivalence ratio ϕ generates more data points in lean and ultra-lean regions, where the flammability is reduced.

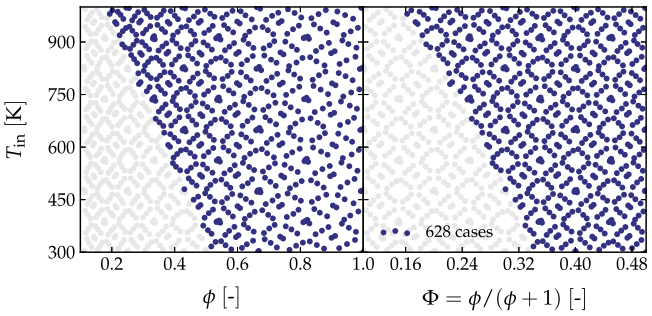

Fig. 1. Data base of pseudo-randomly selected inlet conditions for laminar flame simulations: left and right panels show identical data on (ϕ, T_{in}) and (Φ, T_{in}) planes, respectively. Among 1024 cases, 628 results are viable.

2.3. Flame thickness

Premixed flame thicknesses are assessed based on the temperature profile, where two definitions are used: the standard thermal thickness $\delta_L^0 = \Delta T_{ad}/\max(dT/dz)$ and the total thermal thickness $\delta_L^{t,10-90\%}$, which is calculated based on the distance corresponding to a 10–90% increase of the temperature. The former definition is useful to resolve processes within the inner reaction layer, and is usually smaller than the second definition: in premixed flames, slow reactions taking place in the burnt gases create a long temperature tail [18].

2.4. Characteristic temperatures and values

Characteristic temperatures $T_{i,j}^\star$ and values $v_{i,j}^\star$ are obtained via post-processing of detailed flame structures. $T_{i,j}^\star$ and $v_{i,j}^\star$ are defined based on physical locations of minima and maxima of function values and spatial derivatives, where the following data are considered: (a) species concentrations for k species, (b) their respective net production rates $\dot{n}_k$, (c) heat release $\dot{H}$, and (d) net reaction rates $\dot{\pi}_k$, defined by the law of mass action as the product of reac-

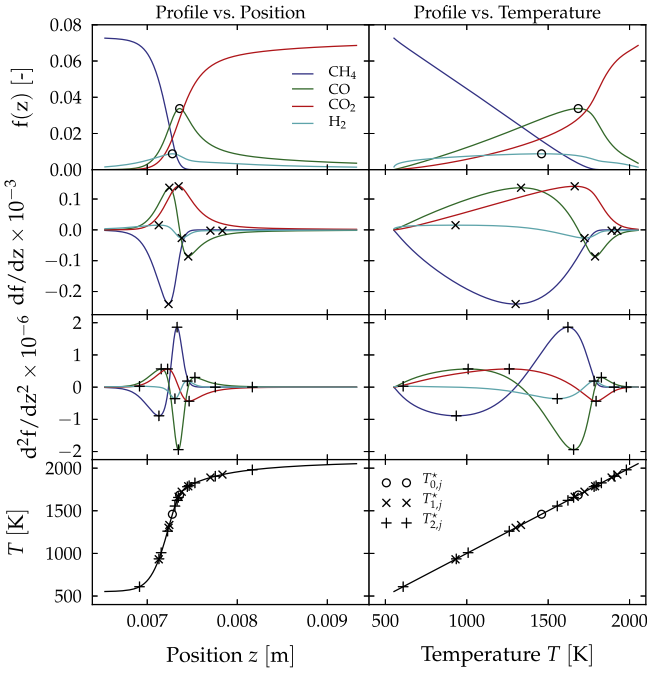

Fig. 2. Definition of characteristic temperatures $T_{i,j}^\star$ based on physical locations of extrema of function values and spatial derivatives.