



Regime identification from Raman/Rayleigh line measurements in partially premixed flames



Sandra Hartl^{a,b,c,*}, Dirk Geyer^b, Andreas Dreizler^d, Gaetano Magnotti^e, Robert S. Barlow^e, Christian Hasse^{a,c}

^a Numerical Thermo-Fluid Dynamics, TU Bergakademie Freiberg, Freiberg, Germany

^b Thermodynamics and Alternative Propulsion Systems, University of Applied Sciences, Darmstadt, Germany

^c FG Simulation of Reactive Thermo-Fluid-Systems, TU Darmstadt, Darmstadt, Germany

^d FG Reactive Flows and Diagnostics, Center of Smart Interfaces, TU Darmstadt, Darmstadt, Germany

^e Combustion Research Facility, Sandia National Laboratories, Livermore, CA, USA

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ABSTRACT

Current methods for combustion regime characterization, such as the flame index, rely on 3D gradient information that is not accessible with available experimental techniques. Here, a method is proposed for reaction zone detection and characterization, which can be applied to instantaneous 1D Raman/Rayleigh line measurements of major species and temperature as well as to results of laminar and turbulent flame simulations, without the need for 3D gradient information. Several derived flame markers, namely the mixture fraction, the heat release rate, and the chemical explosive mode, are combined to detect and characterize premixed versus non-premixed reaction zones. The methodology is developed and evaluated using fully resolved simulation data from laminar flames. The fully resolved 1D simulation data are spatially filtered to account for the difference in spatial resolution between experiment and simulation. Then, starting from just temperature and major species, a constrained homogeneous constant pressure, constant temperature reactor calculation gives an approximation of the full thermochemical state at each sample location along the line. Finally, the chemical explosive mode and the heat release rate are calculated from this approximated state and compared to those calculated directly from the simulation data. As a further test, experimental uncertainty is superimposed onto the filtered numerical data to produce a Raman/Rayleigh equivalent state before running the constrained homogeneous reactor, and results are again compared. After successful tests using the numerical data, the approach is applied to Raman/Rayleigh line measurements from laminar counterflow flames and a mildly turbulent lifted flame. The results confirm that the reaction zones can be reliably detected and characterized using experimental data. Furthermore, the relative importance of premixed and non-premixed reaction zones within the same flame can be qualitatively assessed as demonstrated in the results.

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1. Introduction

Laminar and turbulent combustion processes are often classified globally as either premixed or non-premixed. Premixed flames propagate into a reactant mixture with uniform equivalence ratio, while in non-premixed flames fuel and oxidizer come from opposite sides of the stoichiometric reaction zone. These two limiting cases have been studied extensively and mathematical models have been developed for both classes of flames. In addition, partially premixed flames have been investigated both experimentally and numerically, as reviewed recently by Masri [1]. In most ad-

vanced combustion applications, such as gas turbines, aircraft combustors, or direct-injection engines, complex multi-regime combustion scenarios can occur through partial premixing or recirculation. Thus, a global characterization does not reflect the relevant local conditions which have to be considered. This is especially important for flamelet methods using tabulated manifolds [2–5]. In the present work, we use the term partially premixed to describe all conditions in between the perfectly premixed and perfectly non-premixed limits, and we propose a method to characterize the local reaction zones within partially premixed flames which is in particular suitable for experimental 1D Raman/Rayleigh data.

One feasible way to distinguish between the different combustion modes locally in the context of numerical simulations is to investigate the small-scale interaction between transport and

* Corresponding author.

E-mail address: hartl@stfs.tu-darmstadt.de (S. Hartl).

Nomenclature

Abbreviations

CEMA	chemical explosive mode analysis
CM	chemical mode
DNS	direct numerical simulation
GFRI	gradient-free regime identification
HR	homogeneous constant-pressure constant-temperature reactor
HRR	heat release rate
LES	large eddy simulation
NP	non-premixed
PP	partially premixed
R2P	reactants-to-products
RR	Raman/Rayleigh
WATR	wavelet adaptive thresholding and reconstruction

Subscripts and superscripts

app	approximate-full-state
exp	experimental
fil	spatially-filtered
fuel	fuel
in	inlet
max	maximum
num	numerical
ox	oxidizer
st	stoichiometry
un	uncertainty-added

Greek symbols

λ	eigenvalues
λ_e	eigenvalue with the largest real part
ξ_p	flame index by Domingo <i>et al.</i>
σ	experimental precision
φ	equivalence ratio
φ_{fl}	flammability limits
ϕ	thermochemical variable
ϕ_j	dependent scalar j in thermochemical variable
$\dot{\omega}_i$	source term of species i

Latin symbols

a, b	right and left eigenvectors
a	strain rate
$h_{f, i}$	enthalpy of formation of species i
J	Jacobian
N_S	number of species
p	pressure
Re	real part
sign	signum function
T	temperature
u	velocity
$W_{H,C,O}$	atomic mass of element H, C, O
x, y	axial/lateral coordinate
X_i, Y_i	mole/mass fraction of species i
Z	Bilger mixture fraction

chemistry [6,7]. Within the limits of purely non-premixed combustion, there is a balance between chemical reactions and the transport in the direction of the mixture fraction gradient. Conversely, in the case of premixed combustion, the chemical source terms are balanced by transport along vectors where the mixture fraction is constant. Implicitly using the idea that the direction of mixing determines the local flame structure, several identifiers describing the respective regime have been developed. The flame index G_{FO} proposed by Yamashita *et al.* [8] and the corresponding

normalized flame index ξ_p by Domingo *et al.* [9] are the most commonly used. These indices evaluate the alignment of fuel and oxidizer gradients and thus give an indication of the local mixing in the reaction zone. This state of local mixing can, for example, also be detected in a large eddy simulation (LES) by using a flame sensor [10] based on resolved gradients of major species. Fiorina *et al.* [11] extended the definition of the flame index to account for the alignment of fuel and oxidizer gradients in diffusion-controlled regions of counterflow double flames. A modified version of the flame index for LES was introduced by Domingo *et al.* [12]. A different approach in the context of multi-regime modeling is the combustion regime indicator that was recently proposed by Knudsen and Pitsch [2,6], based on the evaluation and tabulation of gradient quantities. This particular regime indicator considers the local balance of the chemical source term, mixing, and unsteady effects mentioned above. In comparison to the flame index, the results are significantly improved for more complex combustion scenarios. While the idea is intriguing, since it is this interaction of mixing and chemistry that determines the local flame structure, it requires detailed fine-scale information including gradients. Furthermore, Knudsen and Pitsch [2] note themselves that for this specific formulation, it is difficult to compute the second derivative of the progress variable with respect to a flamelet index, which is required for the regime indicator.

The indices and identifiers discussed above have been developed for analysis of direct numerical simulation (DNS) data and for use in numerical modeling. Experimental measurements of the same quantities would be difficult, because most of the definitions are based on the knowledge of 3D gradients of multiple scalars. Rosenberg *et al.* [13] have reported results on the probabilities of finding premixed and non-premixed reaction zones in a turbulent partially premixed combustor, based on a flame index determined from 2D imaging of fluorescent markers. However, 2D projections can misidentify the sign of the scalar product of fuel and oxidizer gradient vectors within a 3D field. Barlow *et al.* [14] used the measured 1D change in mixture fraction across a large jump in temperature (1000 K) as a conditioning variable in their analysis of the transition from premixed to non-premixed burning in the near field of a piloted jet flame. Crossed planar imaging methods have been applied in combination with 1D Raman/Rayleigh measurements to determine instantaneous flame orientation and to approximate 3D gradients in mixture fraction [15] and progress variable [16,17]. However, this limited 3D gradient information is not sufficient to quantitatively determine the flame indices and regime indicators cited above. Consequently, an analysis of the experimental data in terms of the combustion regime has been conducted mostly in connection with simulations. For example, comparing LES results with the experimental data, using conditional averages, provides useful insights with respect to the local flame regime [3,4,18–20]. However, due to the tight coupling of the combustion model with the LES predictions of the fluid flow and the mixing, this cannot be considered as a direct analysis of the experimental data. Another approach is an a priori/prior analysis [3–5], which is feasible for tabulated manifold techniques and can be considered as a more direct approach.

The objective of the present study is to propose and evaluate a regime characterization approach solely relying on spatial 1D Raman/Rayleigh line data for major species concentrations and temperature. The hypothesis underlying this novel approach is that the local thermochemical state depends on the combustion regime and can be considered a “footprint”. Furthermore, as will be demonstrated, knowledge of the local temperature and major species is sufficient to allow approximation of the full thermochemical state, such that the chemical explosive mode [21] and the heat release rate can be calculated. Combinations of these two key flame markers and the mixture fraction are proposed

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