Progress-Variable-Free State-Space Parameterizations for Premixed Combustion

Mohsen Ayoobi, Ingmar Schoegl
Louisiana State University, Mechanical & Industrial Engineering, Baton Rouge, LA, USA.

***Abstract*— Key features of the flame structure remain unchanged throughout the lean and ultra-lean premixed regime, where peak temperatures are a natural parameter. As estimates for peak temperatures can be calculated from local states and transport processes, future expansions to arbitrary reacting flows are envisioned.**

I. Introduction

In state-space modeling with reduced-order chemistry, results of detailed 1D simulations are used to span a manifold in which properties are tabulated based on a small set of parameters. As the resulting chemistry tabulation uses information obtained from detailed reaction mechanisms, full chemistry is implicit to simulation results. A main concern of this approach is a suitable parameterization, and various definitions of parameters and associated manifolds have been proposed in available literature, e.g. Intrinsic Low Dimensional Manifolds (ILDM), various flamelet based approaches (FPV, FGM, MFM, ...), and, more recently, Principal Component Analysis (PCA).

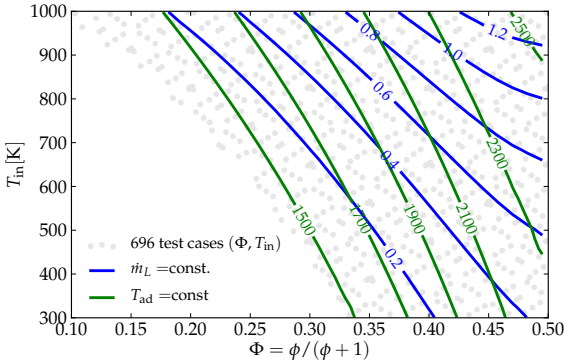

Fig. 1. Contours of constant laminar burning flux $\dot{m}_L$ and adiabatic flame temperature $T_{\rm ad}$ as a function of $T_{\rm in}$ and Φ based on 696 adiabatic flame simulations for lean CH_4/air mixtures (using CANTERA/GRI-Mech 3.0).

II. Methodology

In any state-space modeling approach, the main concern is whether the controlling chemistry manifold captures flame characteristics over a broad range of mixture stoichiometries and reactant temperatures. For the present study, a large number of lean premixed CH_4/air simulations is used to investigate combustion characteristics (Fig. 1). For each simulation, the flame structure is analyzed in terms of species concentrations, net species production rates and heat release. Following a precursor study [2], characteristic temperatures within the inner layer of the flame sheet are defined by minima/maxima of function values, and their first and second derivatives with respect to axial position.

Characteristic temperatures within the flame structure represent *descriptive* information. In order to identify a suitable *minimal* parameterization, the information is plotted in terms of rudimentary parameters that define flame simulations: inlet conditions are specified by (normalized) equivalence ratio Φ and reactant temperature $T_{\rm in}$, whereas laminar burning flux $\dot{m}_L$ and adiabatic flame temperature $T_{\rm ad}$ represent simulation results. Once a suitable parameterization is identified, PCA reveals whether characteristics are valid for a range of similar conditions.

The analysis of the flame structure is based on CH_4/air flames that are both adiabatic and one-dimensional. In the context of arbitrary reacting flows, parameters defining a manifold may not be available locally, and thus require estimates based on *local* mass fractions, temperature and associated transport processes.

III. Results and Discussion

Figure 1 shows 696 test cases where inlet conditions $(\Phi, T_{\rm in})$ follow a pseudo-random Sobol sequence; contours represent simulation results, i.e. $\dot{m}_L$ and $T_{\rm ad}$. For all test cases, characteristic temperatures $T^\star_{i,j}$ are obtained via post-processing of detailed flame structures. Characteristic temperatures for heat release are presented in Figure 2, where insets display $T^\star_{i,j}(\dot{H})$ as a function of Φ, $T_{\rm in}$, $\dot{m}_L$ and $T_{\rm ad}$, respectively. Results illustrate that inlet conditions are ill-suited for a universal parameterization, despite the fact that they constitute the most *convenient* parameterization. In comparison, a parameterization based on $\dot{m}_L$ shows a good collapse of the initial curvature of the heat release, $T^\star_{2,0}(\dot{H})$, which is attributed to a transition from the convection-diffusion dominated preheating layer to the reaction-diffusion dominated active reaction zone. A parameterization based on $T_{\rm ad}$ results in an almost perfect collapse of $T^\star_{i,j}(\dot{H})$, which is a strong indication for $T_{\rm ad}$ being the single-most important parameter characterizing processes within the active reaction zone.

The collapse of characteristic temperatures $T^\star_{i,j}$ for comparable $T_{\rm ad}$ indicates that, except for a scaling factor, species production rates and heat release follow almost

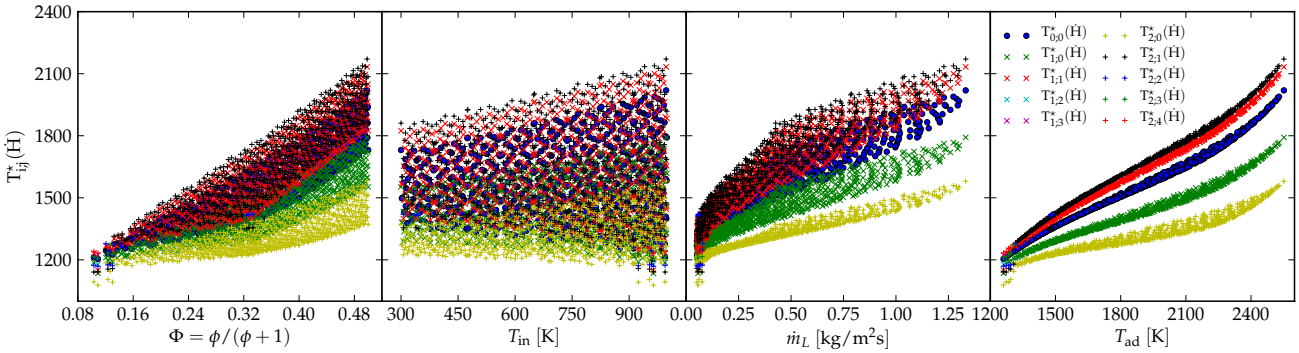

Fig. 2. Comparison of different parameterizations for characteristic temperatures for heat release $\dot{H}$, calculated for 696 test cases (Fig. 1). From left to right, parameterizations use normalized equivalence ratio Φ, inlet temperature $T_{\rm in}$, mass burning rate $\dot{m}_L$, and adiabatic flame temperature $T_{\rm ad}$.

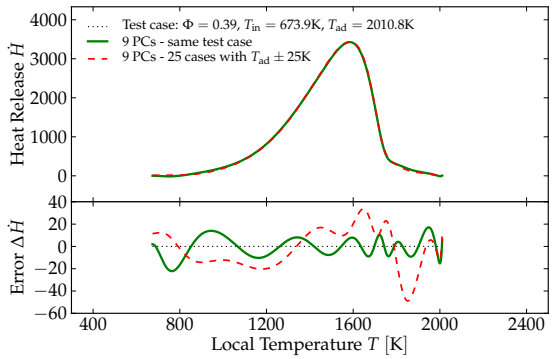

Fig. 3. Principal Component Analysis (PCA): comparison of simulated and recovered heat release $\dot{H}$. Principal components (PC's) are calculated for same test case as well as multiple simulations with comparable $T_{\rm ad}$.

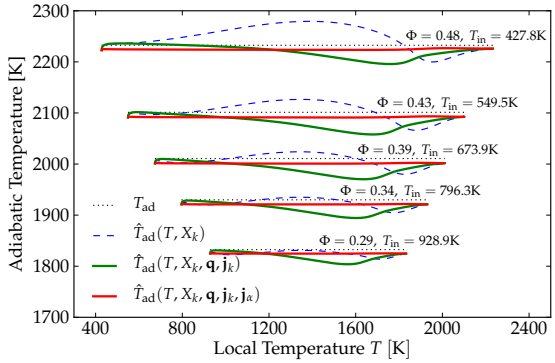

Fig. 4. Estimates for adiabatic temperatures $\hat{T}_{\rm ad}$ based on local temperature T and species concentration X_k, as well as fluxes of heat $\mathbf{q}$, molecular species $\mathbf{j}_k$, and atomic species $\mathbf{j}_\alpha$ [1].

identical progressions. This result implies that a reduced manifold for a description of chemical kinetics can be obtained, where source terms are tabulated based on two parameters: (i) the local temperature T, which captures the position relative to $T^\star_{i,j}$, and (ii) the adiabatic temperature $T_{\rm ad}$ of the flame simulation. Figure 3 compares simulated heat release to heat release recovered from PCA as a function of local temperature. It is evident that $\dot{H}$ is successfully recovered from PC's obtained for multiple test cases with comparable $T_{\rm ad}$, which illustrates the collapse of chemistry characteristics onto a reduced manifold.

PCA results corroborate that net species production rates and heat release collapse based on $T_{\rm ad}$, and thus are governed by a reduced manifold for source terms in suitable transport equations. Since $T_{\rm ad}$ is a non-local characteristic of the local thermo-chemical state, the proposed parameterization required estimates if applied to arbitrary flow fields. In order to obtain accurate estimates for $T_{\rm ad}$, conservation equations for energy and atomic species are integrated along an adiabatic stream tube extending from local conditions to a virtual state far downstream of the flame. Thermodynamic equilibrium yields $\hat{T}_{\rm ad}$ based on estimates for enthalpy and atomic species concentrations; estimates for $T_{\rm in}$ and reactant composition are obtained in a similar fashion [1]. Figure 4 demonstrates that accurate estimates $\hat{T}_{\rm ad}$ are recovered from the local thermo-chemical state, where the consideration of associated transport processes is essential.

IV. Conclusions

A parameterization based on peak temperatures $T_{\rm ad}$ produces an almost perfect collapse of flame characteristics, implying that $T_{\rm ad}$ is a natural parameter for the generation of reduced manifolds for reaction chemistry. In contrast to most other descriptions of manifolds for premixed flames, the current work does not require the definition of a progress variable. Instead, the relative position within the flame is characterized by the local temperature T and an estimate $\hat{T}_{\rm ad}$. It is noted that the procedure applies to arbitrary reacting flows, where corresponding (virtual) 1D premixed flames are obtained by calculating $\hat{T}_{\rm ad}$ from the local thermo-chemical state and associated transport processes.

Acknowledgment

The authors thank for support provided by the LaSPACE program (contract NASA/LEQSF(2010-2015)-LaSPACE).

References

[1] M. Ayoobi and I. Schoegl. Behavior of preheated premixed flames at lean conditions. In *Joint Meeting of the U.S. Sections of the Combustion Institute*, 2013.

[2] J. Gibson, M. Ayoobi, and I. Schoegl. Behavior of preheated premixed flames at rich conditions. *Proc. Combust. Inst.*, 34:997–1005, 2013.