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In-situ tracking of mixture fraction gradient trajectories and unsteady flamelet analysis in turbulent non-premixed combustion

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ABSTRACT

Based on in-situ tracking of gradient trajectories in a direct numerical simulation (DNS), this work combines a structural analysis of a turbulent, temporally evolving syngas jet with an extended flamelet model. This flamelet formulation accounts for curvature-induced flame-tangential transport effects and is formulated in a Lagrangian manner. Using the in-situ trajectory tracking algorithm flamelets are tracked in time and space, and for the first time complete unsteady flamelet histories are reconstructed for further analysis. By extracting all relevant flamelet parameters from the DNS, solutions for the flamelet equations in mixture fraction space with and without flame-tangential transport effects are studied and discussed together with budgets of the equations. Although the overall flamelet structure is compliant with laminar flamelet theory, significant departures from classical flamelet realizations are observed for the scalar dissipation rate. Thus, in addition to flamelets in the classical flamelet regime (no significant flame-tangential transport), additional flamelet structures with non-negligible multi-dimensional effects are observed and both types are analyzed in detail. It is shown how the regime classification is influenced by the relative magnitude of scalar dissipation rate and curvature, two quantities related to the topology of mixture fraction isosurfaces. These surfaces exhibit both regions of high curvature and sheet-like structures. The dynamic interplay of compressive and extensive strain, curvature, and scalar dissipation rate is further studied with a formulation of the scalar dissipation rate equation which accounts for variable thermo-chemical properties. The results illustrate how the topological structure of the mixture fraction field interacts with the flamelet structure.

1. Introduction

In the classical flamelet concept for non-premixed combustion as developed by Peters [1,2], a flamelet represents a one-dimensional structure in the reaction zone of a thin flame. This thin flame sheet assumption results from the insight that chemical time scales in combustion processes are usually fast in comparison to time scales of the flow, such that chemical reactions take place in confined thin layers. With this, and given the fact that the most relevant reactions in non-premixed combustion occur in the vicinity of the stoichiometric mixture of fuel and oxidizer, scalar quantities (e.g. temperature and species mass fractions) can be represented as a function of the mixture fraction described by a one-dimensional equation set. The classical formulation [1,2] of the so-called flamelet equations is self-contained except for the flamelet parameter scalar dissipation rate, which links chemistry to the flow and mixing field. The equations read [1]

$$\rho \frac{\partial Y_i}{\partial t} = \frac{\rho \chi}{2} \frac{\partial^2 Y_i}{\partial Z^2} + \dot{m}_i \,, \tag{1}$$

$$\rho \frac{\partial T}{\partial t} = \frac{\rho \chi}{2} \frac{\partial^2 T}{\partial Z^2} - \sum_{i=1}^{n} \frac{h_i}{c_p} \dot{m}_i + \frac{1}{c_p} \left(\frac{\partial p}{\partial t} + q_R \right) , \tag{2}$$

where Y_i represents the species mass fraction, h_i the species enthalpy, $\dot{m}_i$ the species source term from chemical reactions, T the temperature, Z the mixture fraction, ρ the density, χ the scalar dissipation rate, c_p the heat capacity, p the pressure, and t the flamelet time, respectively. In Eqs. (1) and (2), higher-order terms, which appear in the derivation, are assumed to be negligible [1]. The general characteristic of flamelet and flamelet-like models is a reduction of the representation of chemistry to a reduced set of scalars which makes it an attractive methodology for chemistry tabulation tools that can complement modern CFD codes.

Since the publication of Peters' original work, several authors have applied and expanded flamelet models to describe

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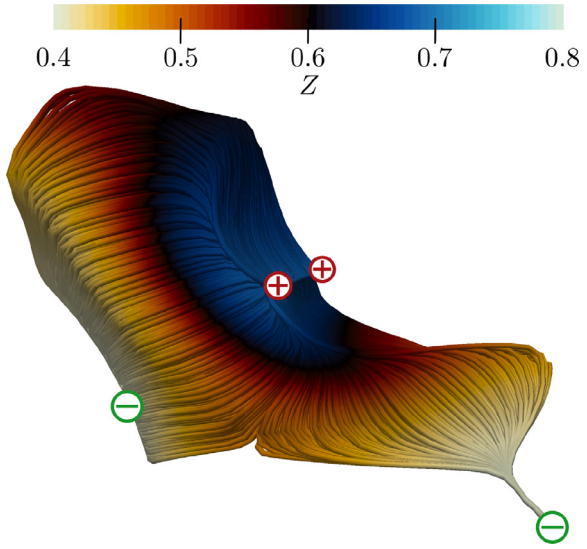

Fig. 1. Illustration of two connected dissipation elements. The red plus and the green minus represent local maximum and minimum, respectively. (For interpretation of the references to color in this figure, the reader is referred to the web version of this article.)

increasingly complex flame configurations. While the classical model is derived for equal diffusivities, Pitsch and Peters [3] developed a formulation that accounts for differential diffusion. Other works suggested extended flamelet formulations for multi-feed combustion [4–6], variable pressure conditions [7], enthalpy effects [8], radiation and enhanced description of pollutant formation [9,10], unsteady effects [11–13], and curvature-induced effects [14–17]. Besides these works, further flamelet models and flamelet-based tabulation strategies were developed, e.g. Flamelet-Generated Manifolds (FGM) [18–20].

Another focal point of Norbert Peters' more recent work was the theory of dissipation elements which represents a novel approach to describe the fine-scale statistics of turbulent flows and turbulent mixing [21–23]. The core principle of this method is the decomposition of a scalar field utilizing its local extremal points, eventually providing information about the underlying topological structure. Dissipation elements have been identified as non-arbitrary, space-filling structures in turbulent scalar fields. They emerge when a gradient trajectory of the scalar field is traced from every point in space in ascending and descending gradient direction until a local extremal point is reached. Dissipation elements are then defined as the ensemble of all gradient trajectories sharing the same local minimum and maximum points, cf. Fig. 1. The theory developed by Wang and Peters [21,22] represents a statistical description of dissipation elements eventually providing information about the scalar dissipation, which is an important parameter for the characterization of turbulent mixing. Since flamelets represent gradient trajectories of the mixture fraction field, the structure-based analysis by Wang and Peters [21,22] is also a promising method for the analysis of turbulent reactive flows. Playing a central role in the flow-chemistry interaction, the scalar dissipation rate and also other relevant quantities (e.g. curvature) might be examined with that approach promoting novel flamelet-based modeling strategies. Note that, unlike laminar flamelets, individual gradient trajectories in a turbulent field generally do not span the whole range between $Z = 0$ and $Z = 1$.

It is the main objective of this study to combine Peters' structure-based analysis of turbulent flows with the latest formulation of non-premixed flamelet equations [17], which also account for non-normal transport processes (i.e. not in the direction of the mixture fraction gradient) and additionally require structure information of the underlying mixture fraction field (such as the curvature). For a detailed analysis of turbulent flamelets, the extended flamelet model is modified to describe flamelets in a Lagrangian manner, similar to the approach by Chan et al. [24], who extracted and investigated turbulent flamelets on a frozen snapshot from the direct numerical simulation (DNS) of a turbulent reacting jet in crossflow. In this work however, flamelets are tracked in time and space facilitated by an in-situ gradient trajectory tracking algorithm. The methodology presented here allows full flamelet histories to be reconstructed from a DNS and provides information on the dynamic interplay of strain, curvature, scalar dissipation, and their effect on turbulent flamelet structures. As DNS case, a spatially evolving non-premixed syngas jet is computed, analogous to a well-established DNS setup [25–29] that exhibits extinction phenomena. This case is revisited with additional in-situ gradient trajectory tracking.

The paper is structured as follows: in Section 2 the DNS setup, the flamelet model, and the in-situ trajectory tracking algorithm are described. In Section 3 the results of the study are presented and discussed. Last, conclusions and a brief outlook are given in Section 4.

2. Numerical methods

In this section the numerical approach for a direct numerical simulation (DNS) of a spatially evolving turbulent syngas jet is presented first. The detailed DNS data is used for the subsequent analyses. Thereafter, an extended flamelet model accounting for curvature-induced effects (non-normal transport), is introduced. Last, to facilitate an assessment of all terms appearing in the flamelet equations, an in-situ gradient trajectory tracking algorithm is presented, that is used for full reconstructions of individual flamelet histories.

2.1. DNS

For our analysis we used the direct numerical simulation code DINO [30–32]. It solves the three-dimensional reactive Navier–Stokes equation using a low Mach number approximation as described in [33]. The governing equations read

$$\frac{\partial}{\partial t}\rho + \nabla\cdot(\rho\mathbf{u}) = 0\,, \tag{3}$$

$$\frac{\partial}{\partial t}\rho\mathbf{u} + \nabla\cdot(\rho\mathbf{u}\mathbf{u}) = -\nabla p + \nabla\cdot\left\{\mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^{\mathrm{T}}) - \frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right\}, \tag{4}$$

$$\rho\frac{\partial T}{\partial t} + \rho\mathbf{u}\cdot\nabla T = \frac{1}{c_p}\left[\nabla\cdot(\lambda\nabla T) - \rho\nabla T\sum_{i=1}^{n} c_{p,i}Y_i\mathbf{V}_{i,j}\right] - \sum_{i=1}^{n}\frac{h_i}{c_p}\dot{m}_i, \tag{5}$$

$$\rho\frac{\partial Y_i}{\partial t} + \rho\mathbf{u}\cdot\nabla Y_i = \nabla\cdot(\rho Y_i\mathbf{V}_i) + \dot{m}_i\,, \tag{6}$$

where $\mathbf{u}$ denotes the velocity vector, μ is the dynamic viscosity, λ describes the thermal conductivity and $\mathbf{I}$ is the identity matrix. The diffusion velocity $\mathbf{V}_i$ is modeled by Fickian diffusion with a correction velocity [34]

$$\mathbf{V}_i = \mathbf{V}^{\mathbf{D,i}} + \mathbf{V}^{\mathbf{C}}\,, \tag{7}$$

where the diffusion velocity $\mathbf{V}^{\mathbf{D,\,i}}$ and the correction velocity $\mathbf{V}^{\mathbf{C}}$ are given as

$$\mathbf{V}^{\mathbf{D,i}} = -\frac{D_i}{X_i}\nabla X_i = -\frac{D_i}{Y_i}\nabla Y_i - \frac{D_i}{\overline{W}}\nabla\overline{W}\,, \tag{8}$$