REACTION ZONE IDENTIFICATION AND CHARACTERIZATION BASED ON RIDGE ANALYSIS

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Abstract
We introduce a novel method for identifying and characterizing reaction zones in combustion. The method is based on the general concept of ridges, i.e., regions where a given spatial field has local directional maxima in directions of its curvature eigenvectors. By identifying the reaction zone with ridges of a suitable reaction strength field allows us to describe the zone in a fully generic way. Firstly, low-dimensional spatial structures that "form the center" of the front can be defined in a natural way. These central regions may locally have different dimension, giving rise to patch-, filament- or sheet-like reaction zones. Secondly, in addition to localizing the central region, one can also infer information about the extent (the "thickness") of the zone from the analysis. This highly generic way of identifying and describing reaction fields can be applied to a wide spectrum of combustion cases, including premixed, non-premixed and partially premixed flames, laminar and turbulent, spanning different regimes (flame-like combustion, broken reaction zones, patch-like structures). As a first demonstration, the method is applied to a Direct Numerical Simulation (DNS) sample of a non-premixed diluted hydrogen/air turbulent flame, using the chemical entropy production rate field as indicator for reaction strength. It is shown that the topology of the central region can strongly differ from the classical "flame sheet" concept. In particular, we find that the filament-type reaction zone geometry is represented frequently in the DNS data set.

Introduction
Many concepts in combustion theory and modeling rely on the notion of a reaction zone [1-3]. A special type of reaction zone is a flame, classically a thin layer where combustion reactions occur, and which propagates by a combination of reaction and diffusive processes. Other types of reaction zone can occur as well, e.g., distributed combustion, or even bulk, volumetric combustion (e.g., after auto-ignition in a homogeneous system).
Existing concepts are widely applied to their respective type of combustion systems (e.g., premixed, non-premixed flames). However, it is unclear how they could be extended to include other systems, like partially premixed flames, or reaction zones which are generally not well described by a flame concept, e.g., zones of auto-ignition.

In view of the rapidly increasing variety of combustion applications, and the tendency to use extreme combustion regimes in technical applications, situations where a clear assignment of a system to one of the traditional paradigms (premixed or non-premixed, flame-like combustion or auto-igniting zones) is no more possible, become increasingly frequent and significant. It is desirable to have a systematic way of describing reaction zones available, which can be applied to a generic combustion system.

In this work, we propose to use the concept of *ridges* for the purpose. Loosely speaking, ridges are regions where a given spatial field has elevated values relative to its neighborhood; a more precise definition based on curvature analysis and directional maxima is given and used in this paper. We apply the ridge concept to a reaction intensity field of a combustion system. The chemical entropy production rate is used as a proxy for the reaction "strength".

The method is applied to three-dimensional DNS of a turbulent, non-premixed hydrogen/air flame. It is found that the reaction zone features aspects that are not covered by the classical notion of a flame-sheet. In particular, when turbulence and reaction interact strongly, the reaction front at some locations is no more a two-dimensional surface, but rather has characteristics of a one-dimensional, filament-like structure. Samples of these structures, which we propose to call flame worms, or shorter *florms*, due to their characteristic appearance, are shown, and some statistics on the front geometry in the DNS data are presented.

The findings can be used to more accurately quantify an effective flame surface of a turbulent flame, and therefore, for improved models of the flame propagation velocity in turbulent combustion. The exact relation of the filament-like structures to turbulence-chemistry interaction, as well as to other one-dimensional turbulence structures, still needs to be investigated.

Methodology

DNS simulation data

A turbulent non-premixed planar flame at atmospheric pressure, where nitrogen-diluted hydrogen (75/25 N2/H2 by mole) flows counter an air stream (79/21 N2/O2 by mole), both at 298 K was simulated by 3D-DNS. Details of the DNS are given in previous papers [4,5]. The data from this DNS was used to apply the concept for reaction zone identification.

Chemical entropy production rate as reaction intensity field

A reaction front is identified in the DNS data as a post-processing step. Several scalars could be employed as reaction front markers, e.g., the chemical source term of some species, or the heat release rate (HRR). However, a single specie's source term does not necessarily monitor the overall chemical activity, and the magnitude of the HRR can be small, even in presence of strong chemical activity, since the effects of exothermic and endothermic reactions may cancel. A quantity that is positive for any chemical activity in a combustion system is the rate of chemical entropy production; the second law of thermodynamics guarantees this positivity.

We used this field in our analysis. Therefore, first the mass-specific chemical entropy production rate (CEPR, in W/(kg· K)) ω_s was computed for every spatial point in the DNS data set. The CEPR is computed by:

$$\omega_S = \sum_{i=1}^{N} \omega_{Y_i} s_i + \frac{\omega_{th}}{T} = \sum_{i=1}^{N} \omega_{Y_i} \left(s_i + \frac{h_i}{T} \right) \quad (1)$$

With index *i* running from 1 to the number of chemical species *N*, ω_{Y_i} denotes the chemical source term of species *i* in a mass-fraction scale, s_i denotes its specific entropy, c_p is the specific heat capacity at constant pressure of the mixture, *T* its temperature, and ω_{th} the temporal rate of temperature change induced by chemical reaction. c_p and s_i are temperature- and composition dependent. The chemical source terms were computed from the species mass fractions, temperature and pressure. using the same reaction mechanism and thermodynamic data that had also been used in the preceding DNS calculations. For illustration, various scalar fields from a sample DNS data set are depicted in Fig.1.

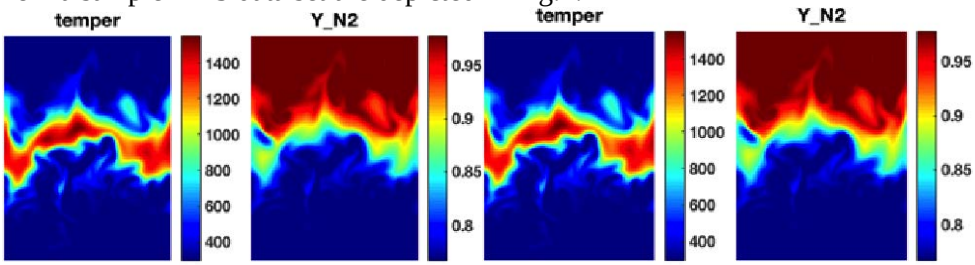

Figure 1. Different scalar fields on the same 2D-slice (size 1 cm × 1.2 cm) from a DNS snapshot. «temper» is the temperature in K, Y_N2 and Y_OH are N_2 and OH masss fractions, and sprod is the chemical entropy production rate ω_s in W/(kg·K). The 2D-slice is perpendicular to the average flame.

It is seen that OH mass fraction (Y_OH) can be large in regions where the local reaction activity is practically zero (e.g., near the right edge of the frames in Fig. 1). The appearance of the ω_s field roughly matches the heat release (not shown here); local differences exist, however. Strong reaction (as indicated by large values of the ω_s field) does not necessarily coincide with high temperatures or large OH mass fractions (Y_OH); large values of T and OH may prevail even if practically no reaction is proceeding (e.g., near the right edge of the frames in Fig. 1). The ω_s field will be used as a proxy for the reaction strength in the following.

Ridge and curvature analysis

A quantitative description of the reaction zone location and its geometry is possible based on the principal curvatures of the three-dimensional CEPR-field.

For this, the Hessian **H** (the matrix of all second spatial derivatives) of CEPR is determined at the spatial point which is to be analyzed. **H** is a real-valued, symmetric matrix, which contains information about the curvature of the three-dimensional ω_S-field. The local structure of the reaction field can be characterized

by an eigenvalue decomposition of the Hessian

$$\mathbf{H} = \mathbf{A}\Sigma\mathbf{A}^{-1} \tag{2}$$

where **A** is a 3×3 matrix containing eigenvectors as columns, and $\sum$ is a 3×3 diagonal matrix of eigenvalues σ_i (i=1,2,3). That is, $\sum$ and **A** have the form:

$$\Sigma = \begin{pmatrix} \sigma_1 & 0 & 0 \\ 0 & \sigma_2 & 0 \\ 0 & 0 & \sigma_3 \end{pmatrix}, \quad \mathbf{A} = \begin{pmatrix} \mathbf{u} & \mathbf{v} & \mathbf{w} \\ | & | & | \end{pmatrix}. \tag{3}$$

The mutually orthonormal vectors **u**, **v** and **w** correspond to directions of principal curvatures of the ω_S-field, and the associated σ_i are the principal curvatures in **u**, **v**, and **w** direction, respectively. The matrices $\sum$ and **A** can be rendered into a form where the eigenvalues are arranged in order of decreasing magnitude ($|\sigma_1|>|\sigma_2|>|\sigma_3|$) along the diagonal; then, the eigenvector **u** corresponds to the direction of strongest curvature (regardless of sign), and eigenvector **w** to the weakest.

A *ridge* is a region where the field has local directional maxima along the eigenvectors [6]. In particular, a point $\mathbf{x}=(x_1, x_2, x_3)$ is on a one-dimensional ridge of the ω_s field if the first two principal curvatures at **x** are negative and ω_s has zero directional derivatives at **x** on the plane spanned by eigenvectors **u** and **v:**

$$\sigma_1 < \sigma_2 < 0 \quad \text{and} \quad \text{grad}_{\mathbf{uv}}\omega_s = 0$$

where $\text{grad}_{\mathbf{uv}}\omega_s$ is the two-dimensional vector formed by the directional derivatives of ω_s along the **u**,**v**-subspace. The zero directional derivative is a necessary, but not sufficient condition for a directional extremum. The negative eigenvalues ensure the local directional maximum. Note again that the eigenvalues are arranged in order of increasing magnitude; for negative eigenvalues, this means that $\sigma_1 < \sigma_2$.

Likewise, **x** is on a two-dimensional ridge (a locally planar structure) if the first principal curvature at **x** is negative and ω_s has a local directional maximum at **x** along **u**: $\sigma_1<0$ and $\text{grad}_{\mathbf{u}}\omega_s = 0$, where $\text{grad}_{\mathbf{u}}\omega_s$ is the directional derivative of ω_s along **u**. Finally, even the degenerate case of a zero-dimensional ridge can occur, namely if **x** is a local maximum in any direction.

Results and Discussion

Depending on the on the different principal curvatures' magnitude, different paradigms for the local geometry of the reaction zone result. Figure 2 sketches these paradigms:

(I) One eigenvalue is dominant over the other two. This corresponds to a two-dimensional reaction front: There is strong curvature of the ω_s field (large magnitude of eigenvalue σ_1) in **u**-direction, and no or only negligible curvature in the other two spatial directions (given by the vectors **v** and **w**). The central region is a two-dimensional object (sheet). The classical two-dimensional flame sheet belongs to this paradigm, with the flame sheet being tangential to the **v**,**w**-plane, and **u** as the local flame-normal direction.

(II) Two eigenvalues are dominant over the third one; the curvature of the ω_s field in two directions (**u** and **v**) is strong, but weak in the third (**w**)-direction. The central region is a one-dimensional object (a curve). This results in a locally cylindrical, filamentary shape of the reaction zone.

(III) All three eigenvalues have the same order of magnitude. Then, the reaction zone has no distinguished local direction, but has a patch-like, roughly spherical shape. The central region is a point.

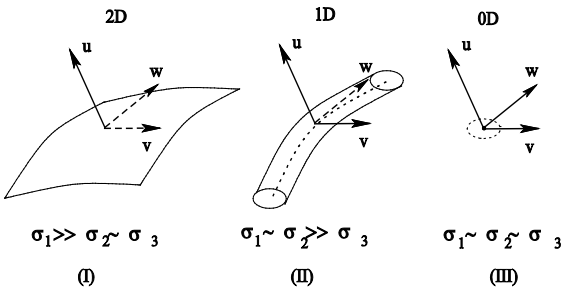

Figure 2. Classification of reaction zone shapes based on magnitudes of principal curvatures, leading to three geometrical paradigms. The dimensions of the underlying ridge structures (central region) are given.

This classification is local and in a combustion system, different paradigms might be encountered at different locations and times. The local shape can be expressed in a quantitative way by defining the ratios $r_{12}=|\sigma_1|/(|\sigma_1|+|\sigma_2|)$ and $r_{23}=|\sigma_2|/(|\sigma_2|+|\sigma_3)|$. Recalling that the σ_i are ordered in decreasing magnitude ($|\sigma_1|>|\sigma_2|>|\sigma_3|$), one can associate the case $r_{12} \sim 1$ to paradigm (I), $r_{12}\sim 0.5$ with simultaneously $r_{23} \sim 1$ to paradigm (II), and $r_{12} \sim 0.5$ with simultaneously $r_{23} \sim 0.5$ to paradigm (III).

In our data set, we frequently found structures corresponding to paradigm (II). An example is depicted in fig. 3.

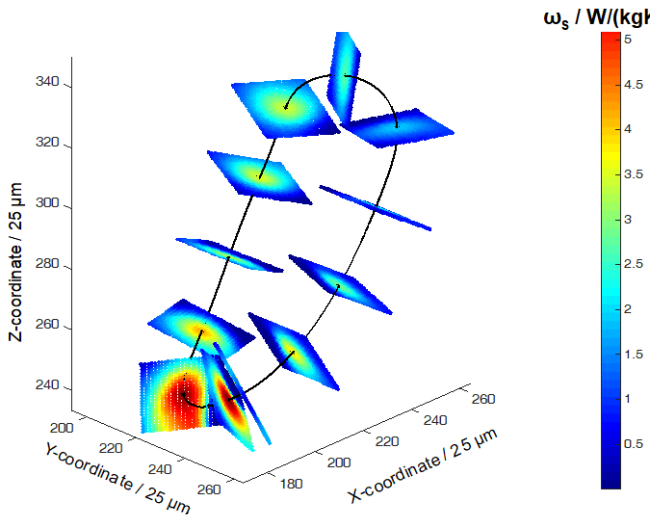

Figure 3. Sample of a reaction structure which is close to paradigm (II) (a flame worm or "florm") in the DNS data set.
Black curve: Tracked central region (a one-dimensional ridge)
Slices: local cut-outs (on planes spanned by the **u** and **v** eigenvectors of the Hessian) of the 3D field ω_S, depicted as false color contour plots.

Conclusions

In this paper, we introduce and demonstrate a generic method for characterizing reaction zones in combustion. It uses the related concepts of *ridges* and curvature analysis of a reaction intensity marker field (the chemical entropy production rate was used for this purpose) to identify two characteristics of the reaction zone: A low-dimensional central region in space, and the spatial extent ("thickness") of the zone. The method is applied to 3D DNS of a turbulent, non-premixed hydrogen/air flame. It is found that the reaction zone in the DNS features aspects that are not covered by the classical notion of a flame-sheet. In particular, when turbulence and reaction interact strongly, the reaction front at some locations is no more a two-dimensional sheet, but rather has characteristics of a one-dimensional, filament-like structure. These structures, which we propose to call flame worms, or shorter *florms*, are expected to bear considerable significance for turbulent combustion modeling. In particular, considering the inclusion of the *florm*-like reaction zone paradigm might extend models relying on flame surface density.

Acknowledgements

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