Flame front characterization based on ridge analysis

R. Schießl, V. Bykov
Institut für Technische Thermodynamik, Karlsruher Institut für Technologie (KIT)
Karlsruhe, Germany

1 Introduction

The mathematical modeling and numerical investigation of turbulent combustion phenomena comprises very complicated fields of combustion theory and applications [1,2]. There is increasing activity towards numerical investigations of turbulent flames using Direct Numerical Simulations (DNS) [3] and analysis of their results [4]. The data reveal that, especially in turbulent combustion, phenomena appear that challenge the classical models for combustion. Also, as combustion science turns towards new applications, also more generic concepts of reaction and turbulence interaction are desired. We introduce an approach that has potential to fulfill this role: The ridge concept is used for characterizing the reaction zone in combustion. Ridges, defined as regions on which a spatial field has directional local maxima along directions given by the eigenvectors of the local Hessian [7], generalize the concept of critical points [8], which already have been used to describe geometrical aspects of flames. The method is highly generic with respect to the kind of fuel/oxidizer-combination, the premixing state (non/partially/fully premixed), the degree of mixture homogeneity within the reaction zone, and the level of flow-turbulence interaction. It therefore can help to overcome limitations of existing reaction zone concepts, which are mostly designed and valid for particular cases only.

The ridge concept is applied to a suitable field representing the local reaction source term. It can identify the location of the reaction zone center, and an appropriate local coordinate frame, local orientation and its shape. Additional analysis of the principal curvatures of the source term field in the vicinity of the center then characterizes the geometrical extent (the "thickness") of the reaction zone.

Mathematically, the ridge concept allows three qualitatively different reaction front shape paradigms. One of these corresponds to the classical flame sheet, which is well represented in combustion systems and theoretical models. The other two paradigms represent less familiar shapes, namely filamentary and patch-like reaction zones.

We apply the concept to three-dimensional DNS-data of turbulent, non-premixed diluted hydrogen/air combustion. It is found that the reaction front based on the ridge-concept may deviate significantly from the stoichiometric iso-surface. Furthermore, at some locations, the zone does not form a two-dimensional surface, but rather has characteristics of a one-dimensional, filament-like structure. Conditional statistics on reaction zone characteristics obtained by the ridge concept are presented.

Correspondence to: robert.schiessl@kit.edu

The results are significant, for instance, for more accurate quantification of an effective flame surface of a turbulent flame, and therefore, for improved models of the flame propagation velocity in turbulent combustion.

2 DNS data

DNS simulations of turbulent non-premixed combustion at atmospheric pressure, where nitrogen-diluted hydrogen (75/25 N_2/H_2 by mole) flows counter an air stream (79/21 N_2/O_2 by mole), both at 298 K, were used for the study [5]. This type of flame is particularly interesting for our purpose, because it features several complexities, which make the description and modeling of the reaction zone with conventional methods quite challenging. First, the strong fuel dilution causes chemical reaction to be quite weak, allowing turbulence and the enhanced molecular transport it causes to interact strongly with the reaction zone. Consequently, while burning globally stable, the flame features events of local extinction and re-ignition. Furthermore, although the flame is nominally non-premixed, the high diffusivity of hydrogen causes it to attain at least partially also premixed character. The strong turbulence/chemistry interaction also creates a reaction zone that significantly deviates from the classical notion of a folded flame sheet. The DNS simulations were carried out by ISUT, Magdeburg University, by their highly parallel, three-dimensional code DINOSOARS [5], a low Mach number solver using a 6th order finite difference scheme for spatial derivatives and a 4th order explicit Runge-Kutta scheme for time integration. This DNS data set has been introduced in [6].

The reaction zone is identified in the DNS data as a post-processing step. To represent the reaction source term, we use the chemical entropy production rate (ω_s). For illustration, various scalar fields, including ω_s (labeled "sprod" in the diagram) from a sample DNS data set are depicted in Fig.1, on two-dimensional slices cut out of the 3D data set. Comparison of the fields illustrates how the reaction zone shows up for different scalars. 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 reaction region also does not coincide with the locus of stoichiometric mixture fraction (points where Y_N2 is near 0.88).

3 Ridge concept and its implementation

Ridges [7] are regions on which a scalar field has directional local maxima along subspaces spanned by the eigenvectors $\boldsymbol{u}$, $\boldsymbol{v}$, $\boldsymbol{w}$ of the Hessian **H** (matrix of second spatial derivatives of the field). **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,

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

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

$$\Sigma = \begin{pmatrix} \sigma_1 & 0 & 0 \\ 0 & \sigma_2 & 0 \\ 0 & 0 & \sigma_3 \end{pmatrix}, \quad \mathbf{A} = \begin{pmatrix} \mathbf{u} & \mathbf{v} & \mathbf{w} \\ | & | & | \\ | & | & | \end{pmatrix}. \tag{2}$$

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 ∑ 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.

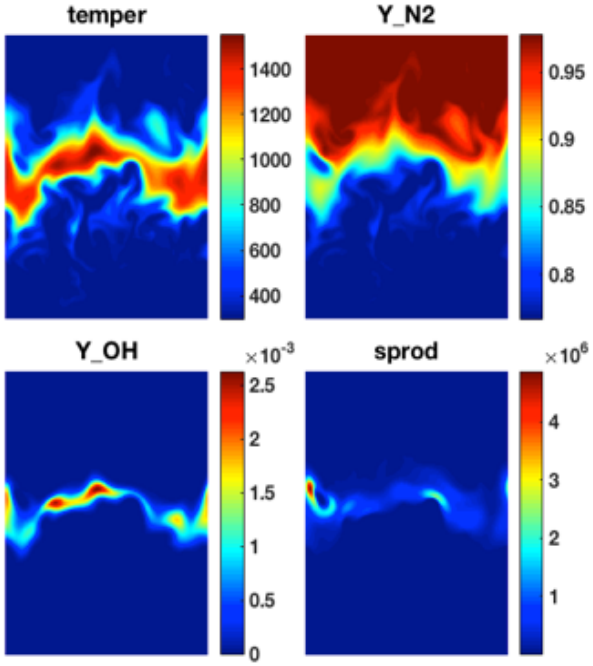


Figure 1. Different instantaneous scalar fields on a 2D-slice (size 1 cm × 1.2 cm) from a DNS snapshot. «temper» is the temperature in K, Y_N2 and Y_OH are the mass fractions of N_2 and OH, respectively, and «sprod» is the chemical entropy production rate in W/(kg·K). The 2D-slice is perpendicular to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

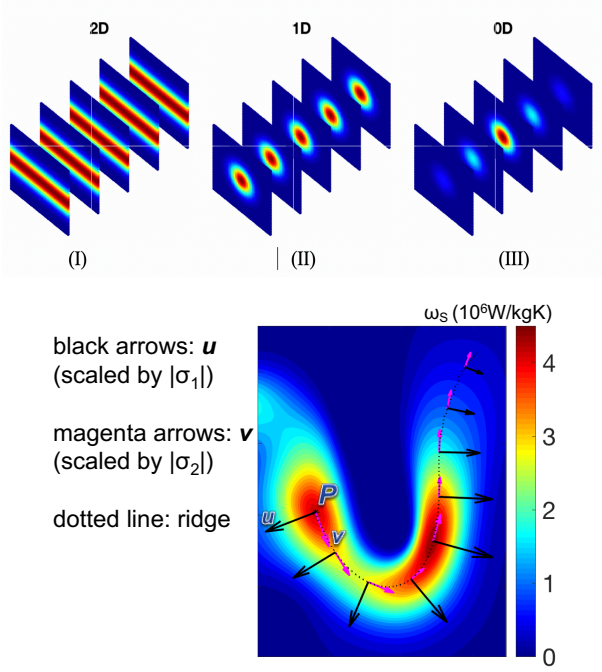


Figure 2. **Top**: classification of reaction zone shapes based on magnitudes of principal curvatures, leading to three geometrical paradigms, the dimensions of the underlying ridge structures are given on top; **Bottom** - a 2D cut from an instantaneous 3D DNS reaction source field (colored contours) with a ridge.

In particular, a point $\boldsymbol{x}=(x_1, x_2, x_3)$ is on a one-dimensional ridge of the ω_s field if the first two principal curvatures σ_1, σ_2 at $\boldsymbol{x}$ are negative and ω_s has zero directional derivatives at **x** on the plane spanned by eigenvectors $\boldsymbol{u}$ and $\boldsymbol{v}$**:**

$$\sigma_1 < \sigma_2 < 0 \tag{3}$$

and simultaneously

$$\nabla_{\boldsymbol{uv}}\, \omega_s = 0, \tag{4}$$

where $\nabla_{\mathbf{uv}}\, \omega_s$ is the two-component vector formed by the directional derivatives of ω_s along the $\boldsymbol{u}$,$\boldsymbol{v}$-subspace, which can be expressed by

$$\nabla_{\boldsymbol{uv}}\, \omega_s = \nabla \omega_s \cdot (\boldsymbol{u}, \boldsymbol{v}) \tag{5}$$

where $\nabla\omega_s = (\partial_x\omega_s, \partial_y\omega_s, \partial_z\omega_s)^T$ is the conventional gradient and $(\boldsymbol{u}, \boldsymbol{v})$ is a matrix with 3 rows and 2 columns formed by the eigenvectors $\boldsymbol{u}$ and $\boldsymbol{v}$. The "·" is used to here to denote matrix-vector multiplication.

The value zero for the directional derivative is a necessary, but not a sufficient condition for a directional extremum. By additionally requiring strictly negative eigenvalues σ_1 and σ_2 (eq. (3)), a local directional

maximum is ensured. Note that the eigenvalues are arranged in order of increasing magnitude; for negative eigenvalues, this implies that $\sigma_1 < \sigma_2$. The points along a one-dimensional ridge are close to paradigm (II).

Likewise, **x** is on a two-dimensional ridge (a locally planar structure) if the first principal curvature σ_1 at **x** is negative and ω_s has a local directional maximum at **x** along **u**:

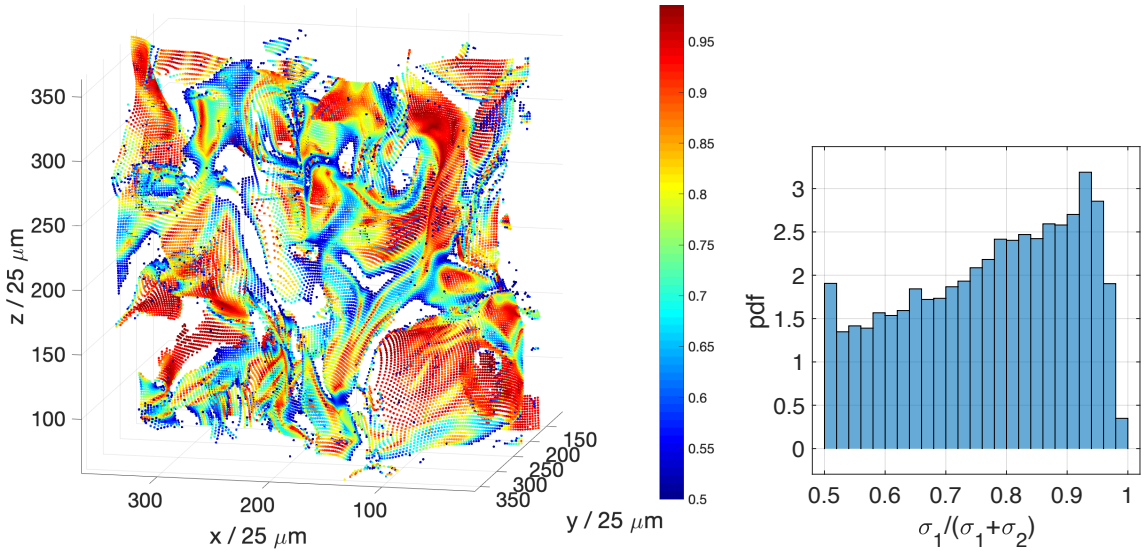
$$\sigma_1<0 \text{ and } \mathrm{grad}_{\mathbf{u}}\omega_s = 0 \qquad (6)$$

where $\mathrm{grad}_{\mathbf{u}}\omega_s$ is the directional derivative of ω_s along **u**. Points on a two-dimensional ridge are close to paradigm (I).

Finally, even the degenerate case of a zero-dimensional ridge can be defined, namely if **x** is a local maximum in any direction, paradigm (III).

To summarize, one can associate paradigms (I), (II), (III) from Fig. 2 (top) with a two-, one- and zero-dimensional ridge, respectively. This highlights the close connection of the curvature analysis and the ridge concept.

4 Results



(a) **(b)**

Figure 3. (a) - Three-dimensional ridge analysis of the DNS, displaying the ratio $r_{12}=|\sigma_1|/(|\sigma_1|+|\sigma_2|)$ as a scatter plot vs. the 3 spatial dimensions (b) - bar-plot representing the pdf of the ratio r12. r12=.5 corresponds to paradigm II („worm-like“), r_{12}=1 is paradigm I (the classical flame sheet).

Figure 3 (a) shows an example a three-dimensional ridge analysis of the DNS as a scatter plot. For this figure, points from the DNS data were collected that are directional maxima of the source field (in the sense outlined in section 3), and that additionally feature source terms that are at least 1% of the maximum source term. These points form a ridge, and therefore, according to our proposed concept, are part of the reaction zone. The points are colored by their ratio $r_{12}=|\sigma_1|/(|\sigma_1|+|\sigma_2|)$, as indicated in the legend. According to section 3, r_{12}=0.5 (bluish colors) corresponds to paradigm 2, r_{12}=1 (red) corresponds to paradigm (I) (the classical

flame sheet). It is seen that there are significant coherent structures along the reaction zone that are close to r_{12}=0.5, as apparent by the blue streaks in Fig. 3(a). These regions deviate from the notion of a flame sheet.

Figure 3(b) shows statistics of the quantity r_{12} as a probability density function (pdf). It is seen that, while more points are close to r_{12}=1 (flame sheet) than close to 0.5 (the "worm-like" paradigm (II)), paradigm (II) is still represented significantly in the data.

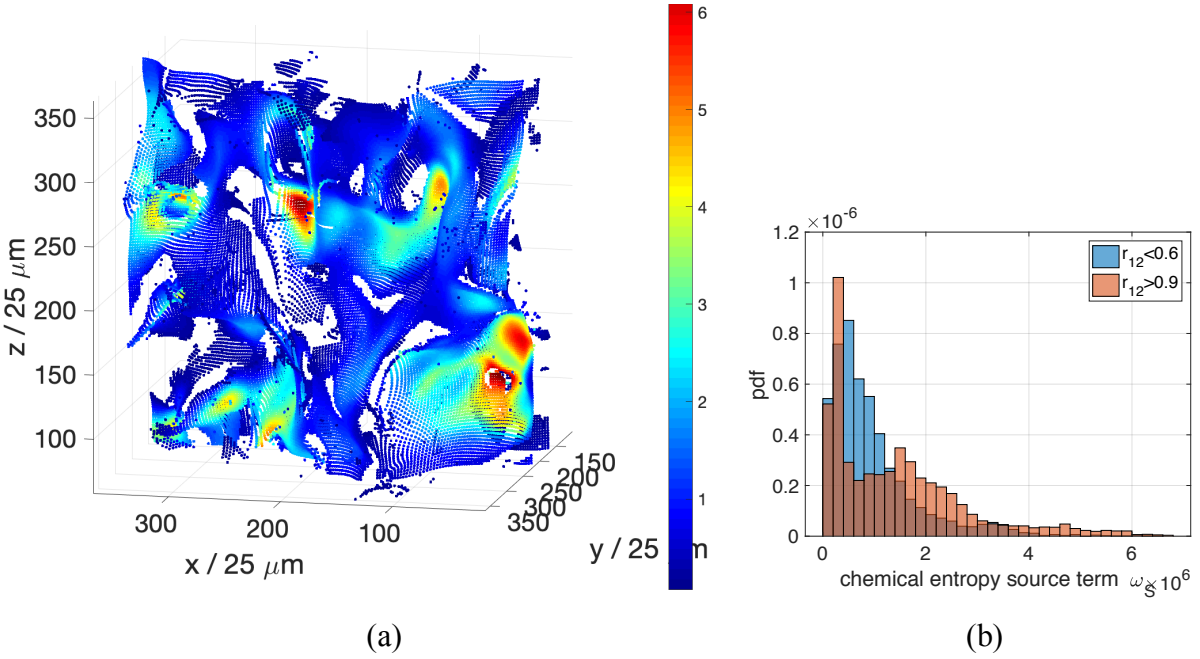


Figure 4. (a) Three-dimensional ridge analysis of the DNS, displaying the underlying chemical source term (in this case, the chemical entropy production rate) as a scatter plot vs. the 3 spatial dimensions. (b) Bar-plots representing the pdfs of ω_s, conditioned on r_{12} <0.6 (blue, close to paradigm (II), „worm-like") and r_{12} >0.9 (red, paradigm (I), the classical flame sheet).

Figure 4 (a) shows the same ridge points as Fig. 3 (a), but now colored by their chemical source term. The source term field selected (ω_s) is the same like the one that was used for the ridge analysis. It is seen that points on the ridge differ strongly in their source term, covering values from near 0 to more than 6×10^6 W/(kg·K). To find out whether the source terms on parts of the ridge that correspond to paradigm (II) differ from ones for paradigm (I), Fig. 4 (b) shows pdfs, conditioned on r_{12} <0.6 (blue, close to paradigm (II), „worm-like") and r_{12} >0.9 (red, paradigm (I), the classical flame sheet). It is apparent that the pdfs are significantly differ between the two paradigms. Beside their different geometric significance, the two paradigms also describe different dynamics of the combustion system.

5 Conclusions

A method for reaction zone identification and analysis based on the concept of ridges was introduced. Ridges provide a natural and generic way for this task. A distinction and systematic classification of structural paradigms (reaction sheets, "worms" or patches) becomes possible. A statistical analysis reveals that for the studied DNS case, "tube" or "worm"-like reaction structures were frequently observed, and that a significant portion of combustion appears not as a classical flame-sheet, but in worm-shaped reaction zones.

This classification may open alternative viewpoints on modeling of reaction-diffusion structures, which can be valuable especially in highly turbulent flames. It was found that the reaction front based on the ridge-concept may deviate significantly from e.g. the stoichiometric iso-surface. These observations can be used, for instance, 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.

Acknowledgments

The authors acknowledge the support by the Deutsche Forschungsgemeinschaft (DFG) within the DFG-RFBR grant BY 94/2-1 (DFG) / 17-53-12018 (RFBR).

References

[1] Warnatz J, Maas U, Dibble RW. (2004). Combustion, 4, Springer-Verlag, Berlin Heidelberg.
[2] Echekki, T., Mastorakos, E. (2011). Turbulent Combustion Modeling, Advances, New Trends and Perspectives, Springer-Verlag, Berlin, Heidelberg, New York.
[3] Chen J.H. (2011). Petascale direct numerical simulation of turbulent combustion – Fundamental insights towards predictive models, Proc. Combust. Inst. 33: 99.
[4] Bennett, J.C., Krishnamoorthy, V., Liu, S., Grout, R.W., Hawkes, E.R., Chen, J.H., Shepherd, J., Pascucci, V., Bremer, P.-T. (2011). Feature-based statistical analysis of combustion simulation data, IEEE Transactions on Visualization and Computer Graphics 17: 1822.
[5] Abdelsamie, A., Fru, G., Oster, T., Dietzsch, F., Janiga, G., Thévenin D. (2016). Comput. Fluids 131: 123.
[6] Schießl, R., Bykov, V., Maas, U., Abdelsamie, A., Thevenin, D. (2017). Implementing multi-directional molecular diffusion terms into Reaction Diffusion Manifolds (REDIMs), Proc. Comb. Inst. 36(1): 673-679.
[7] Eberly, D., (1996). *Ridges in Image and Data Analysis*, Series on Computational Imaging and Vision, Kluwer Academic Publishers, September ISBN 0-7923-4268-2.
[8] Griffiths, R. A. C., Chen, J. H., Kolla, H., Cant, R. S., & Kollmann, W. (2015). Three-dimensional topology of turbulent premixed flame interaction. Proc. Comb. Inst. *35*(2): 1341–1348.