Implications of the alignment of dissipative fluxes for reduced combustion modeling

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Abstract — **3D DNS data of turbulent non-premixed and premixed flames are analyzed with respect to the dimension of the local subspace spanned by different scalars' gradients. It is found that the gradients are closely confined to a two-dimensional subspace of 3D geometrical space. This observation opens new perspectives for reduced combustion modeling. The REDIM approach is considered and used to interpret the results of the DNS-based gradient estimates.**

I. Introduction

The interaction of diffusive transport processes with chemical reaction is an important phenomenon in combustion. Since diffusive transport is controlled by the strength and spatial alignment of scalars' gradients, a detailed analysis of these characteristics of the gradient field can promote a better understanding of combustion phenomena, and can also aid the development of improved reduced models for combustion. A typical assumption underlying reduced models is that the local dissipative fluxes of all scalars are aligned with one spatial direction. This direction can be given, for instance, by the gradient of mixture fraction in the classical non-premixed flamelet model [1]. The key advantage of this simplification is that diffusive processes can be described by one single parameter [1,2].

However, the diffusive fluxes are vector-valued quantities, and their full description therefore requires a specification of both magnitude and direction, especially in very complicated flows such as turbulent combustion. It is important to assess the influence of multi-dimensional molecular transport processes and the role of the transport with respect to the definition of reliable reduced description of combustion processes. To this end, a method for gradient analysis of local gradient vectors for different scalars, is introduced and applied to Direct Numerical Simulation (DNS) data sets of a turbulent nonpremixed combustion scenario. The extent of the directional scatter of gradients (and therefore, of diffusive fluxes) is found to be considerable. It is found that the scatter is not fully random, but approximately restricted to only two spatial dimensions.

II. Analysis of DNS Data

A. Data and methodology

DNS data were provided by ISUT at Magdeburg University. Details of the employed DNS method are given in [5], therefore, only a short account is given here. The DNS feature a non-premixed atmospheric pressure scenario where diluted N_2/H_2 (75%/25% by mole) counter-flows with an air stream (79% N_2, 21% O_2 by mole), all at 298 K. Detailed chemistry [6] is used with a simplified Le=1 assumption for the transport. The latter was employed, in this first analysis, to avoid the additional complications associated with effects like differential diffusion, thermo-diffusion etc. A velocity field from artificial turbulence, with Re_l=500 (based on integral length-scale) is used. The resulting turbulent flame featured local extinction, but was globally burning stably, as is indicated by the temporal evolution of the heat release rate. In this study, the direction that best represents the trend of the different local gradient vectors is identified. For this, the matrix G^{norm} formed from the normalized local scalar gradient vectors is decomposed according to the singular value decomposition (SVD, [7]) into the product of three matrices A, S and B according to:

$$G^{norm} = A \cdot S \cdot B^T .$$

The vectors in matrix A can be interpreted as a local basis of 3D geometrical space which is optimally aligned with the vectors in G^{norm} (as exemplified in fig.1, left diagram); matrix A, therefore, can be thought of as a dissipation-aligned coordinate frame. The singular values σ_i contained in S represent the importance of the corresponding basis vector in A for the description of the vectors in G^{norm}. Since $\sigma_1 > \sigma_2 > \sigma_3$, there is a hierarchical ordering of the vectors u, v, w in A. Fig. 1 shows, as an exemplary result, a temporal snapshot from the DNS-analysis, the fields of temperature (center) and of the ratio $\sigma_2/(\sigma_1+\sigma_2)$ (right part of the image) in a typical turbulent flame region. The maximally possible value for this ratio is 0.5, and the flame features extended regions where values close to this limit are reached. For describing the directions of gradient vectors, at least two directions are needed. Remarkably, however, the ratio $\sigma_3/(\sigma_1+\sigma_2+\sigma_3)$ remains small everywhere in the DNS data set: the gradient vectors in the DNS data set do not "use" the third spatial dimension, even though it would be available.

B. Incorporation into the REDIM concept

By applying the unitary transformation $A^T \cdot G^{norm}$, the coordinates of the variables' gradients in the standard (x,y,z)-coordinate frame (as extracted from the DNS data) are transformed into the coordinates in the dissipation-aligned (u,v,w) coordinate system. These (u,v,w)-based coordinates of gradients can be used as hierarchically structured gradient estimates amd employed in the REDIM equation to construct the manifold (see [3] for more details).

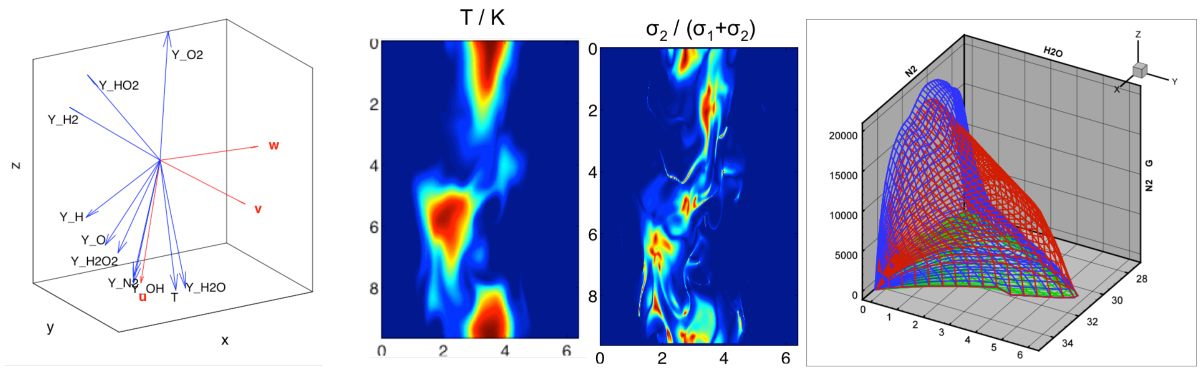

Fig. 1 Left: A three-dimensional example of directions of scalar gradients from one point in the DNS data set. Gradient vectors of different species scatter approximately within a two-dimensional space. Center left: 2D-cut through the temperature field from the DNS sample, showing a turbulent flame (false colour scale from 300 K to 1350 K). Center right: the ratio $\sigma_1/(\sigma_1+\sigma_2)$ of singular values (false colour scale from 0 to 0.5) from the SVD of the local normalized gradient vectors. In some regions within the flame, the ratio is close to the maximum possible value of 0.5, indicating extremely strong local directional scatter of scalar gradients. The x- and y-axes in the central and right diagram are in scales of mm. Right: DNS-derived gradient estimate used for computing a REDIM.

Namely, in the orthogonal local coordinate system (u, v, w) the gradients $grad_{u,v,w}(\psi)$ are estimated (see Fig. 1, on the left) and the information about the parameter $grad_{u,v,w}(\theta)$, gradients can be transferred to the local coordinates.

III. Conclusions

The dimension of the subspace spanned by local diffusion fluxes in a non-premixed turbulent combustion scenario is studied using 3D DNS data. In the considered flame configuration, the local diffusion fluxes of different species display considerable directional scatter. Remarkably, however, they reside approximately within a two-dimensional subspace of three-dimensional geometrical space.

This indicates that at least two spatial directions would be needed for a full description of the local diffusive fluxes. Our analysis of DNS data also offers a local hierarchical decomposition of the directions for diffusive transport, based on a singular value decomposition of the local gradient vectors. This establishes a hierarchy of the local gradients (and therefore also of the diffusive fluxes) into a principal direction and secondary directions along which diffusive transport proceeds.

These observations have potential significance for simplified computational models, since here mostly only a locally one-dimensional diffusive transport is provided for. In order to assess the significance of the multi-dimensional transport for turbulent combustion regimes, the results of the DNS data analysis are interpreted by applying the REDIM approach [3]; moreover, it can be used as an input to improve the REDIM with respect to the transport processes. Thus, it is shown how a DNS-based gradient estimates can be incorporated into the REDIM method. Thus, one-, two- and three-dimensional gradient estimates can generically be accounted for [3,4].

Comparing REDIMs with gradient estimates based on one- and two-dimensional dissipation, it is found that, at least for the conditions of the DNS considered here, the two-dimensional dissipative transport is of negligible influence on the overall behavior of the reaction-diffusion system. However, for stronger turbulence or when more detailed models for dissipative transport are used, the multi-dimensional transport might gain importance. The methodology developed in this study can and will be applied to data with higher turbulence and with more complex transport models in future work.

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References

[1] N. Peters, Proc. Comb. Inst. 21 (1987) 1231–1250.

[2] J.A. van Oijen, L.P.H de Goey, Combustion Theory and Modelling (CTM) 6 (2002) 463–478.

[3] V. Bykov and U. Maas, Combustion Theory and Modelling (CTM) 11(6) (2007), 839–862.

[4] V. Bykov and U. Maas, Proc. Combust. Inst. 34 (1) (2013) 197–203.

[5] Abdelsamie, A. and Thévenin, D., in Direct and Large-Eddy Simulation IX, (Fröhlich, J., Ed.), Dresden, 62-63 (2013).

[6] Maas, U. and J. Warnatz, Combustion and Flame 74 (1988) 53-69.

[7] G. Golub and C. van Loan 1996. Matrix Computations: Johns Hopkins University Press.