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The (mis)alignment of diffusive fluxes in turbulent combustion: DNS analysis and treatment in the Reaction-Diffusion Manifold (REDIM) model

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Abstract
3D DNS data of decaying turbulent non-premixed flames are analyzed with respect to the mutual alignment of the local scalar’s gradients. The gradients of species are not aligned with one single direction, but mostly point in different directions, approximately scattering within a 2D space. The significance of this scatter for the REDIM approach is studied by employing DNS-based gradient estimates as a basis to compute REDIMs. REDIMs obtained with a “conventional” and with a 2D-gradient estimate are compared. The difference is insignificant, indicating that for the current conditions of the DNS (low turbulence with a Taylor Reynolds number Reₜ ≤ 30), the multi-directional nature of dissipative transport is not important.

Introduction
The interaction of diffusive transport processes with chemical reaction is an important phenomenon for combustion. Improved insight into the mutual coupling of reaction and diffusive processes is a key for better understanding of combustion phenomena. The term representing diffusive transport via dissipative fluxes in the detailed scalar transport equations finds its correspondence, in various forms, also in reduced, approximate models for combustion.

Typically, in such models the same local direction for the transport of all scalars is assumed. This might be termed “one-dimensional transport” - the local dissipative fluxes of all scalars are aligned with one spatial direction. This direction is, for instance, given by the gradient of mixture fraction in the classical non-premixed flamelet model [1]. Thus, most studies in this field predominantly base their analysis or description solely on the magnitude of transport processes. 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 specification of both magnitude and direction. The importance of the full description increases with the extent of “non-parallelity” of the local gradients.

In this context, it is interesting to check the parallelity of the diffusive fluxes in a practical combustion scenario. Ideally, experiments in flames could be used for this. However, the analysis would require instantaneous, spatially resolved three-dimensional fields of multiple scalars (ideally, of all species, pressure and temperature) to be measured. This is beyond the currently available capabilities of measurement equipment.

In this work, we consider instead data samples from three-dimensional Direct Numerical Simulations (DNS) of turbulent non-premixed flames. The mutual alignment of diffusion flux vectors of different variables is studied. To this end, a method for gradient analysis, including a quantification of the misalignment of local gradient vectors for different scalars, is introduced and applied to the DNS data set. The extent of the directional scatter of gradients (and therefore, of diffusive fluxes) is found to be considerable. Remarkably, the scatter is not fully random, but approximately restricted to only two spatial dimensions.

This indicates that at least two 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 (SVD) 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.

In order to assess the significance of the multi-dimensional transport for turbulent combustion regimes, the results of the DNS data analysis are incorporated into the REDIM approach [3] as DNS-based gradient estimates. In the REDIM method, one-, two- and three-dimensional gradient estimates can generically be accounted for [3, 4]. REDIMs are then computed for identical boundary conditions, but with the different gradient estimates. Both the observed principal and secondary gradient components from the DNS analysis are used, either separately or in combination. Differences between the two REDIMs are discussed.

Methodology

2.1. DNS data
DNS results were obtained by mean of the highly parallel, three-dimensional in-house DNS code “DINOSOARS”. DINOSOARS is a low Mach number
Fig. 1 Left: Some synthetic normalized gradient vectors (simplified example in two dimensions), and the first column \( u \) (principal direction) and second column \( v \) (secondary direction) of the matrix \( Y \) resulting from the hierarchical decomposition via SVD. Right: A three-dimensional example of actual gradients from the DNS data set. Normalized gradient vectors of different species and temperature (as indicated by the labels) are shown along with the three principal direction vectors \( u, v, w \). The gradients are not well-aligned, but scatter approximately within a two-dimensional space.

2.2. Analysis of gradients

The DNS data set delivers spatio-temporal fields of (among others) the state variables temperature \( T \) and \( n_s \) species mass fractions \( Y_i \) \((i = 1, \ldots, n_s)\), comprising a \( n_s = (n_s+1) \)-dimensional state vector \( \psi = (T, Y_i) \) at each spatial and temporal point. To analyze the strength and relative orientation of the \( n_s \) different scalars’ gradients, for each time step of the DNS data set, 5000 random points were selected from regions where the heat release rate was at least a specified fraction of the global maximum heat release. Several thresholds were used in different runs of the analysis, ranging from \( 10^{-6} \) to \( 10^{-1} \). At each one of these points, the 3D spatial gradients for all scalars were determined. The resulting gradients were arranged into a 3-by-\( n_s \) gradient array \( G \), in which columns correspond to variables and rows correspond to spatial directions \((x, y, z)\). Normalizing all columns of \( G \) to 1 then yields a normalized version \( G_{\text{norm}} \) of \( G \). We are interested in the mutual (mis)alignment of the gradient vectors in \( G \) or \( G_{\text{norm}} \), as opposed to the “overall” direction of the gradients dictated by the local flame orientation. To determine and remove the overall trend, a local coordinate frame that is aligned with the dissipation field is constructed, and the analysis then focuses on the components of the gradients in this aligned frame.

Several methods exist for constructing such a locally aligned coordinate system. For instance, the gradients of selected species or other state variables may be used as a basis for the coordinate system. The classical non-premixed flamelet model [1] employs the gradient of the mixture fraction for this purpose.

In this paper, we take a different approach, searching for the direction that best represents the trend of the different local gradient vectors. For this, the matrix \( G_{\text{norm}} \) is decomposed according to singular value...
decomposition (SVD, [7]) into the matrix product of three matrices A, S and B according to:

\[ G^\text{norm} = A \cdot S \cdot B^T, \]

where the superscript “T” denotes matrix transposition. The column vectors of the 3x3 matrix A form an orthonormal basis in geometrical space, which is optimally aligned with the directions of the local gradient vectors in \( G^\text{norm} \). The two-dimensional example in Fig. 1 (left) illustrates this, while the diagram on the right shows a genuine example for the vectors extracted from a point of the DNS. The first column (named u) of A is optimally aligned with the direction of the gradient vectors. The second column (v) in A optimally describes the direction of the gradient vectors after their u-component has been removed, while the third column (w) of A represents the direction that is least represented by the gradient vectors. The column vectors in A = (u v w) therefore constitute a “dissipation-aligned” orthogonal coordinate system, which additionally offers a natural hierarchy of gradient directions.

The matrix S is a diagonal matrix with real positive entries \( \sigma_i \), (called singular values) which appear sorted (from large to small) along the diagonal (top to bottom right) of S. The \( i \)-th singular value represents the importance of the \( i \)-th column vector in A for the description of the vectors in \( G^\text{norm} \). Since \( \sigma_1 \geq \sigma_2 \geq \sigma_3 \), this reflects the hierarchical ordering of the vectors u,v,w in A. Figure 2 shows, as an exemplary result from the DNS data 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. Significant regions exist in the flame where the ratio approaches the value 0.5 (the maximum possible value, since \( \sigma_2 \leq \sigma_1 \), i.e., where the local gradient vectors are close to the maximally possible misalignment.

For our analysis, the Matrix B is of minor interest.

By applying the unitary transformation \( A^T \cdot G^\text{norm} \), the coordinates of the variables’ gradients in the standard (x,y,z)-coordinate frame are transformed into the coordinates in the dissipation-aligned (u,v,w) coordinate system. These (u,v,w)-based coordinates of gradients will be considered in the sections below.

2.3. Modified REDIM method

In order to illustrate how multi-dimensionality of the system gradients can be accounted for, an overview of the REDIM method will be shortly given in this subsection (see e.g. [3,4] for details). The original system of equations governing the reacting flow can be cast in vector form in coordinate free formulation as the following

\[ \frac{\partial \psi_i}{\partial t} = \text{F} (\psi) - \bar{\psi} \text{grad} \psi + \frac{1}{\rho} \text{div}(D(\psi) \text{grad} \psi) \]  

(1)

This system describes the evolution of the thermochemical state vector \( \psi = (\psi_1,...,\psi_n) \) in time and in physical space, where the \( \psi_j \) represent such quantities as the pressure of the mixture \( \rho \), the enthalpy \( h \) and chemical species’ specific mole numbers \( Y_i / M_i, i=1,...,n_3 \) (mass fractions divided by molar masses). \( F \) represents the chemical source term, \( \bar{\psi} \) is velocity vector, \( \rho \) is the density and \( D \) is the general diffusion matrix. A reduced model can be created by assuming existence of internal relations (correlations) between the variables of the system (1) such that the detailed system evolves within a low-dimensional surface (manifold) in the state space spanned by the \( \psi_j \). This manifold then can be explicitly defined and described as

\[ M = \{ \psi = \psi(\theta); \theta = (\theta_1,...,\theta_m) \}, m << n. \]  

(2)
The REDIM equation can be used to find the manifold (surface) resulting from the invariance relations (see e.g. [3,4,8]), by using some initial solution and estimates of the detailed system’s gradients as

\[
\begin{align*}
\left[ \frac{\partial \psi(\theta,t)}{\partial t} \right] &= \left( I - \psi^T \psi_n \right) [F(\psi(\theta)) + T(\psi(\theta))] \\
\psi(\theta,0) &= \psi_0(\theta) \\
T(\psi(\theta)) &= \frac{1}{\rho} \text{div}(D(\psi(\theta))\psi_\theta(\theta)\text{grad}\theta)
\end{align*}
\]  
(3)

In this approach, the molecular transport term describing the fluxes $\text{div}(D(\psi)\text{grad}\psi)$ explicitly depends on the detailed system’s gradients calculated on the manifold

\[
\text{grad}\psi(\theta) = \psi_\theta(\theta) \text{grad}\theta
\]  
(4)

Hence, the information on the gradients and their dependence on the reduced variable $\theta$ must be specified in any solution of Eq. (3) can be calculated. Note that the reduced system’s state space – the manifold in Eq. (2) – is defined by only two processes (reaction and diffusion, see e.g. [3] and Eq. (3)). The gradients in Eq. (4) have to be incorporated consistently with the problem’s boundary- and initial conditions. In order to illustrate how the multi-dimensional transport can be accounted for, the transport term is simplified by assuming a constant diagonal diffusion matrix and a Cartesian coordinate system

\[
T(\psi) = \text{div}(D(\psi)\text{grad}(\psi)), \\
D(\psi) = d \cdot I \Rightarrow T(\psi) = d \text{div}(\text{grad}(\psi))
\]  
(5)

Thus, the simple Laplacian diffusion term in 3D can be written as:

By using the gradient estimate as described in subsection 3.2 below and the definition of the Laplace operator, the transport term (transversal to the tangential space of the manifold), Eq. (5) on the manifold can be further simplified to:

\[
\begin{align*}
\text{grad}(\psi) &= \begin{bmatrix}
\text{grad}_x(\psi) \\
\text{grad}_y(\psi) \\
\text{grad}_z(\psi)
\end{bmatrix} \\
\Rightarrow T(\psi) &= d \begin{bmatrix}
\psi_{1,xx} + \psi_{1,yy} + \psi_{1,zz} \\
\psi_{2,xx} + \psi_{2,yy} + \psi_{2,zz} \\
\vdots \\
\psi_{n,xx} + \psi_{n,yy} + \psi_{n,zz}
\end{bmatrix}
\end{align*}
\]

Hence, the gradients of the parameter on the manifold are only needed to employ the REDIM equation and integrate Eq. (3).

These gradients can be found from the DNS data analysis: In the orthogonal local coordinate system $(u, v, w)$, the gradients $\text{grad}_{u,v,w}(\psi)$ are estimated (see Fig. 3), and the information about $\text{grad}_{u,v,w}(\theta)$ can be transferred to the local coordinates according to Eq. (4). E.g. for the u-direction, it reads

\[
\begin{align*}
\text{grad}_u(\psi) &= \psi_\theta \text{grad}_u(\theta) \Rightarrow \\
\text{grad}_u(\theta) &= \psi_\theta \text{grad}_u(\psi(\theta))
\end{align*}
\]  
(7)
Results

3.1. Gradient statistics

The directions of gradients corresponding to different variables often scatter strongly (cf. Fig 1). The leftmost diagrams in Fig. 2 show, as a representative data set, the temporal development of the $u$-, $v$- and $w$-components of $\text{grad}(T)$ in the flame, as obtained from the DNS data analysis described in section 2.2. The $v$- and $w$-components are plotted vs. the $u$-component. Each of the 9 sub-diagrams refers to one time step of the DNS simulation, as indicated in the labels (times are given in units of 0.1 microseconds). For the initial, laminar flame (time 0), the $v$- and $w$-components are zero, reflecting the fact that the gradient of temperature is perfectly aligned with the first principal direction (the $u$-direction). In fact, for early times, all scalars’ gradients are oriented in the same direction, therefore only the $u$-component is non-zero for all gradients. This corresponds to the case of one-dimensional dissipation, stemming from the one-dimensional flame-based scalar fields used to initialize the DNS. With increasing time, the $v$-component becomes increasingly important. After 0.36 ms (a time slightly larger than the initial turbulent large eddy turnover time scale, $1.125 \, \tau_\Lambda$), the magnitudes of $u$- and $v$-components become comparable, and two spatial directions now essentially dominate the diffusive transport. Note that the $v$-component can show the same magnitude as the $u$-component also for large values of the gradients; the directional scatter is therefore by no means only a spurious phenomenon that occurs only at small, insignificant gradients.

The third ($w$-) component of the gradient, however, remains small at all timesteps. Although the third dimension (pointing in $w$-direction) is available in principle, it is practically not represented in the data. Therefore, dissipation here is an essentially two-dimensional phenomenon.

3.2. 1D and 2D gradient estimates

As a result of the SVD-analysis, $u$, $v$ and $w$ components of gradients are available for 5000 DNS data points, along with the mass fractions of $N_2$ and $H_2O$ and the corresponding values ($\theta_1$, $\theta_2$). The data points $(\text{grad} \psi_k, q_1, q_2)$ ($q=u, v, k=N_2, H_2O$) approximately describe two-dimensional surfaces; numerical
Dissipative processes in two-dimensional geometrical spaces can be estimated and incorporated in the DNS-based solution gradients. The DNS data analysis provides gradient estimates for different cases, together with some stationary solutions of counterflowing flames with different strain rates. For the blue mesh, only 1D dissipation (using grad\(_u\)) is accounted for; the green mesh is also for 1D dissipation, but with only grad\(_\theta\), considered in Eq. (7). The red mesh shows the manifold when both grad\(_u\) and grad\(_\theta\) are considered in the REDIM evolution equation, Eq. (3). Significant differences are apparent when only the second direction is accounted for (even for main radicals like O or H\(_2\)O\(_2\)), the maximum concentration is slightly overestimated by the green mesh, see Fig. 4, while the differences between blue and red are moderate. At the same time, Fig. 4 (on the right) shows that the chemical source terms evaluated on the REDIM match much better for both the minor as well as for major species. It additionally gives credits to the 1D model in the example considered here. Namely, it can satisfactorily be described using only one-dimensional dissipation, along the first (u-) direction.

### Conclusions

The mutual alignment of the local diffusion fluxes of different state variables (temperature and species) in a non-premixed turbulent combustion scenario has been studied using 3D DNS data. In the considered flame configuration, the local diffusion fluxes of different species display considerable directional scatter, while residing approximately within a two-dimensional subspace of the three-dimensional geometrical space. Such a two-dimensional nature of diffusion fluxes is not accounted for in most simplified combustion models. The significance of the multi-dimensional transport for model reduction was then studied using a REDIM-approach, which naturally allows incorporating these effects. Different REDIMs for identical boundary conditions, but with different dimensionality of the DNS-based gradient estimate were computed and compared. The differences, while noticeable, are quite small.

We conclude that, for the conditions of the DNS considered here (low turbulence level), the two-dimensional dissipative transport is of negligible influence concerning the overall behavior of the reaction-diffusion system. However, for stronger turbulence (Re\(_<\)60, leading to high mixing and dissipation rate) or when more detailed models for molecular transport are used, the multi-dimensional transport might rapidly gain importance as an influencing factor. The methodology developed in this work will be applied to corresponding data with higher turbulence and with more complex diffusion models in the near future.

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