Multi-dimensional transport: DNS analysis and incorporation into the Reaction-Diffusion Manifold (REDIM) method

R. Schießl, V. Bykov and U. Maas
Institut für Technische Thermodynamik, Karlsruher Institut für Technologie (KIT)
Engelbert-Arnold-Straße 4, Geb. 10.91, 76131 Karlsruhe

1 Introduction

The significance of diffusive transport in combustion has long been recognized. The term representing diffusive transport via dissipative fluxes in the detailed Navier-Stokes equations finds its correspondence, in various forms, also in reduced, approximate models for combustion. An important feature is that simplified models often assume the same local direction for the transport of all scalars. This situation could 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.

The advantage of this simplification is that diffusive processes can be described by one single number, which describes the local "strength" (magnitude) of the diffusive flux [1, 2]. However, it is unclear how this restriction to one dimension affects the model accuracy.

In this paper, the mutual alignment of the local diffusion fluxes of different state variables in a non-premixed turbulent combustion scenario is studied using 3D DNS data. It is found that the diffusive fluxes (as inferred from spatial gradients) of different species display a considerable directional scatter. This scatter is not fully random, but approximately restricted to a two-dimensional subspace of the three-dimensional geometrical space.

These observations may be important in the context of computational models for a simplified description of reaction-diffusion systems. To assess this importance, the significance of the multi-dimensional transport for the REDIM-approach [3] is studied. In the REDIM method, one- two- and three dimensional gradient estimates can generically be accounted for [3,4]. REDIMs for identical boundary conditions, but with different dimensionality of the gradient estimate are computed and compared. The difference, while noticeable, is overall quite small. This indicates that, at least for the conditions of the studied flames, the two-dimensional diffusive transport has little influence on the overall behavior of the reaction-diffusion system.

Correspondence to: robert.schießl@kit.edu

2 Methodology

2.1. DNS data

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 [5] is used with a simplified *Le* = 1 assumption for the transport. The computation domain had a size of 3.4 x 10 x 6.8 mm^3, with a spatial resolution of 25 micrometer, and the time step for the numerical solution was 0.1 microseconds. The DNS were initialized with species- and temperature profiles from a laminar one-dimensional flame simulation, broadcast onto the 3D DNS geometry. A velocity field from artificial turbulence, with Re_l=500 (based on integral length-scale), u'=2,1 m/s was overlaid. The resulting turbulent flame featured local extinction, but was globally burning stably, as is indicated by the temporal evolution of the heat release rate.

2.2. Analysis of gradients

To analyze the strength and relative orientation of 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 certain fraction of the global maximum heat release. Several fractions were used in different runs of the analysis, ranging from 10^{-6} to 10^{-1}.

For each scalar ψ_i (temperature and 9 species, H_2, O_2, H_2O, H_2O_2, HO_2, OH, H, O, N_2) at one point, the spatial gradients were determined. The resulting gradients were arranged into a 3-by-10 (3-by-n_ψ in general) gradient array G, such that columns of G correspond to variables and rows correspond to spatial directions (x,y,z). Normalizing all columns of G to 1 then formed a normalized version G^{norm} of G.

We are interested in the mutual (mis-)alignment of the gradient vectors in G, 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. The gradients of selected species or

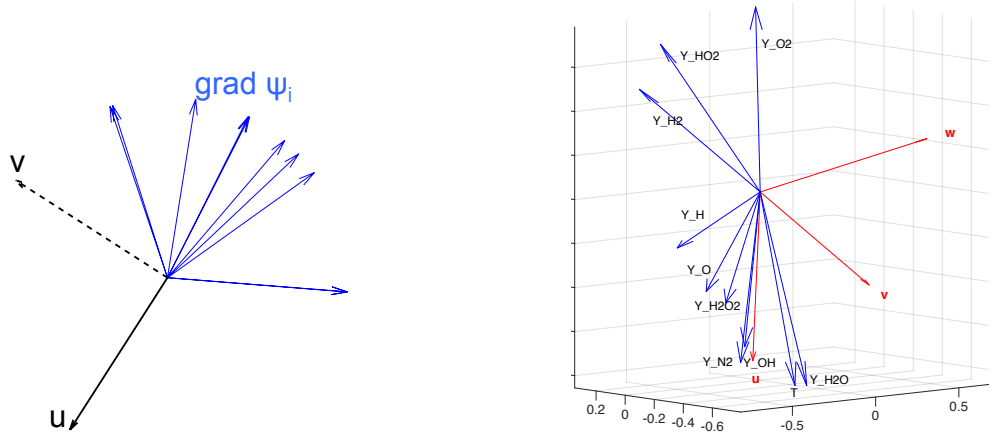

Fig. 1 Left: Some synthetic normalized gradient vectors (simplified example in two dimensions), and the first column u and second column v of the matrix Y resulting from the SVD-analysis. Right: A three-dimensional example of actual gradients from the DNS data set. Gradient vectors of different species are not well-aligned, but scatter approximately within a two-dimensional space.

other state variables may be used as a basis for the coordinate system. For instance, in the classical non-premixed flamelet model, the gradient of mixture fraction is used for this purpose.

In this paper, we take a different approach, which automatically includes all state variables. For this, the matrix G^{norm} is decomposed according to the singular value decomposition (SVD, [7]).

$$\mathsf{G}^{\text{norm}} = Y \cdot S \cdot V'$$

The column vectors of the 3x3 matrix Y form an orthonormal basis of geometrical space, which is optimally aligned with the directions of the local gradient vectors in G^{norm}. The two-dimensional example in Fig. 1 (left) illustrates this, while the right diagram shows a genuine example for the vectors extracted from a DNS. The first column (named u) of Y is optimally aligned with the direction of the gradient vectors. The second column (v) optimally describes the direction of the gradient vectors after their u-component has been removed, and the third column (w) represents the least significant direction. The column vectors in Y = (u v w) therefore establish a "dissipation-aligned" orthogonal coordinate system, which additionally offers a natural hierarchy of directions.

By applying the unitary transformation $Y' \cdot \mathsf{G}^{\text{norm}}$, 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 will be considered in the following.

2.3. Modified REDIM

The original system of equations governing the reacting flow can be cast in the vector form in coordinate free formulation as the following [1,2]

$$\frac{\partial \psi}{\partial t} = F(\psi) - \vec{v}\,\text{grad}\,\psi + \frac{1}{\rho}\text{div}\left(D(\psi)\text{grad}\,\psi\right) \tag{1}$$

This system describes the evolution of the thermo-chemical state vector $\psi = (\psi_1,...,\psi_n)$ in time and in physical space, where the ψ_j represent such quantities as the pressure of the mixture p, the enthalpy h and chemical species' specific mole numbers $w_i / M_i, i = 1,...,n_s$ (mass fractions divided by molar masses). F represents the chemical source term, $\vec{v}$ is velocity vector, ρ is the density and D is the general diffusion matrix. A reduced model can be created assuming approximate relations between the variables of the system (1) such that they define a low-dimensional surface (manifold) in the state space spanned by the ψ_j. This manifold then can be defined as

$$M = \{\psi = \psi(\theta), \quad \theta = (\theta_1,...,\theta_m)\},\ m << n\,. \tag{2}$$

The REDIM methods is based on the solution of the REDIM equation following from the invariance relations (see e.g. [8]) as

$$\begin{cases} \dfrac{\partial \psi(\theta,\tau)}{\partial \tau} = \left(I - \psi_\theta \psi_\theta^+\right) \cdot \left[F(\psi(\theta)) + \dfrac{1}{\rho}\text{div}\left(D(\psi(\theta))\psi_\theta(\theta)\text{grad}\,\theta\right)\right] \\ \psi(\theta,0) = \psi_0(\theta) \end{cases} \tag{3}$$

In this approach the molecular transport term describing the fluxes $\text{div}(D(\psi)\text{grad}\,\psi)$ explicitly depends on the spatial gradient on the manifold

$$\text{grad}\,\psi(\theta) = \psi_\theta(\theta)\text{grad}\,\theta \tag{4}$$

Hence, information on the gradients and their dependence on the reduced variable θ must be specified before the stationary solution of Eq. (3), which represents the manifold Eq. (2) used to reduce the system, can be calculated. Note that the reduced system's state space Eq. (2) is defined by only two processes (reaction and diffusion, see e.g. [4] and Eq. (3)), while the advection influences the manifold by the gradients. Eq. (4) that has to be incorporated consistently with the problem's boundary- and initial conditions. In order to show transparently how the multi-dimensional transport can be accounted for, the transport term

$$\text{T}(\psi) = \text{div}\left(D(\psi)\,\text{grad}(\psi)\right), \quad D(\psi) = d \cdot I \Rightarrow \text{T}(\psi) = d\,\text{div}\left(\text{grad}(\psi)\right) \tag{5}$$

is simplified by assuming a constant diagonal diffusion matrix and considered in Cartesian coordinate system. Thus the simple Laplace diffusion term in 3D can be cast:

$$\mathrm{grad}(\psi)=\begin{pmatrix} \mathrm{grad}_x(\psi) & \mathrm{grad}_y(\psi) & \mathrm{grad}_z(\psi) \\ | & | & | \end{pmatrix} \Rightarrow \mathrm{T}(\psi)=d\begin{pmatrix} \psi_{1,xx}+\psi_{1,yy}+\psi_{1,zz} \\ \psi_{2,xx}+\psi_{2,yy}+\psi_{2,zz} \\ \ldots \\ \psi_{n,xx}+\psi_{n,yy}+\psi_{n,zz} \end{pmatrix} \tag{6}$$

By using the gradient estimate as described above and the definition of the Laplace operator, the transport term (transversal to the tangential space of the manifold) Eq. (6) on the manifold can be further simplified to:

$$\mathrm{T}(\psi(\theta))=d\,\psi_{\theta\theta}(\theta)\circ\mathrm{grad}(\theta)\circ\mathrm{grad}(\theta)=$$

$$=d\left(\mathrm{grad}_x(\theta)^T\cdot\psi_{\theta\theta}(\theta)\cdot\mathrm{grad}_x(\theta)+\mathrm{grad}_y(\theta)^T\cdot\psi_{\theta\theta}(\theta)\cdot\mathrm{grad}_y(\theta)+\mathrm{grad}_z(\theta)^T\cdot\psi_{\theta\theta}(\theta)\cdot\mathrm{grad}_z(\theta)\right)$$

Hence, the gradients of the parameter on the manifold are only needed to employ the REDIM equation (solution of Eq. (3)). These can be found as results of the DNS data analysis. Namely, in the orthogonal local coordinate system (u,v,w) the gradients $\mathrm{grad}_{(u,v,w)}(\psi)$ are estimated (see Fig. 3) and the information about the parameter $\mathrm{grad}_{(u,v,w)}(\theta)$ gradients can be transferred to the local coordinates according to Eq. (4), e.g. for the u-direction it reads

$$\mathrm{grad}_u(\psi)=\psi_\theta\,\mathrm{grad}_u(\theta)\rightarrow\mathrm{grad}_u(\theta)=\psi_\theta^+\,\mathrm{grad}_u(\psi(\theta)). \tag{7}$$

3 Results

3.1. Gradient statistics

The directions of gradients corresponding to different variables scatter strongly (cf. Fig 1).
Figure 2 shows, as a representative data set, the temporal development of the u, v and w components of grad(T) in the frame, as obtained from the 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 a time step of the DNS simulation, as indicated in the labels. For the initial, laminar flame (time 0), the v- and w-

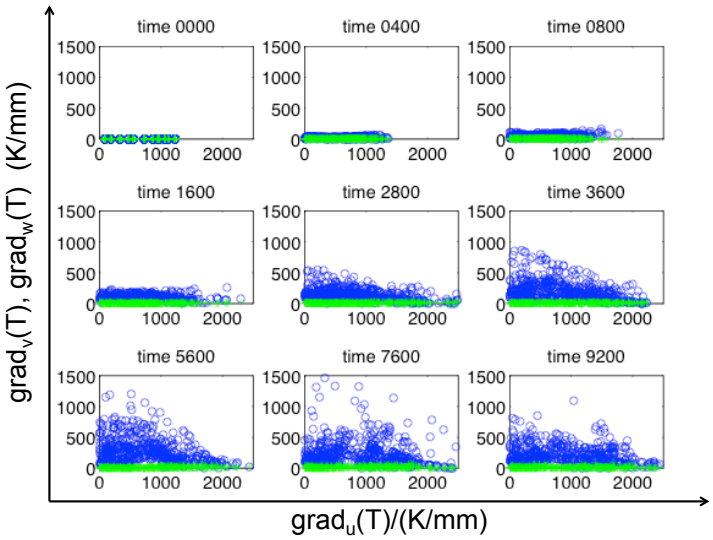

Fig. 2 Temporal development of the u-,v- and w-components of grad(T). Time steps are given in units of 0.1 microseconds.

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. With increasing time, the v-component becomes increasingly important. After 3600 time units (1 unit corresponds to 0.1 microseconds), 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 be in the same magnitude as the u-component also for large values of the gradients; the directional scatter is therefore not a spurious phenomenon that occurs only at small, insignificant gradients. The third (w-) component of the gradient, however, remains small at all timesteps. The dissipation therefore, 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 (θ_1, θ_2). The data points ($grad_q\psi_k$, θ_1, θ_2) (q=u,v , k=N_2,H_2O) approximately describe two-dimensional surfaces; numerical representations of these surfaces were computed on a rectangular grid in the REDIM coordinates (θ_1,θ_2) by taking a distance-weighted average of $grad_q\psi_k$ at each grid point. Figure 3 shows the resulting surfaces for the u- and v-components of grad N_2 and grad H_2O.

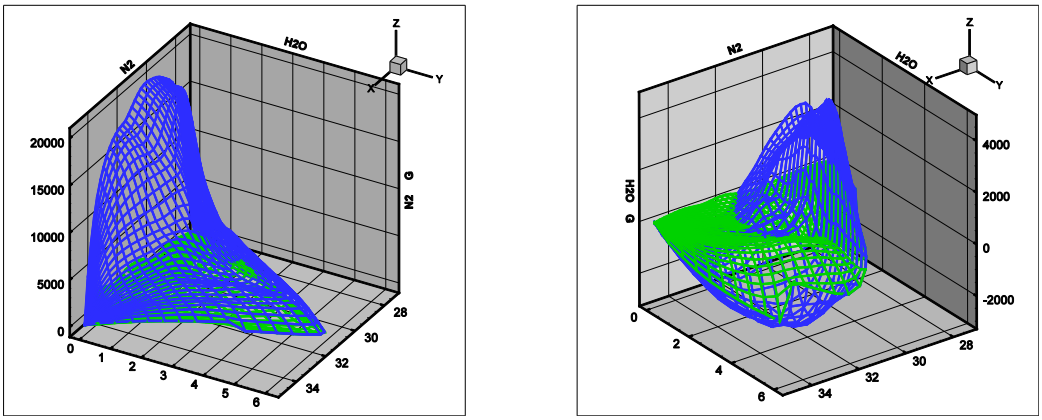

Fig. 3. DNS-based gradient estimates (u- and v-components) on the REDIM manifold as a function of (N_2, H_2O). Blue – $grad_U$ N_2 and H_2O, green – $grad_V$ of N_2 and H_2O.

3.3. REDIM with 1D and 2D transport

From the DNS data analysis, we observe that the dissipative processes in the considered example are essentially two-dimensional (in the sense of section 3.1). Therefore, the third term in Eq. (7) is negligible, while the second term does have some noticeable contribution (see Fig. 3, green mesh). Figure 4 shows the resulting REDIMs for three different cases. For the blue mesh, only 1D dissipation (along $grad_u$) is accounted for; the green mesh is also for 1D dissipation, but with only $grad_v$ considered in Eq. (7). The red mesh shows the manifold when both $grad_u$ and $grad_v$ 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 H or H_2O_2, the maximum concentration is overestimated by the green mesh, see Fig. 4), while the differences between blue and red are moderate. We conclude that the example considered here can satisfactorily be described using only one-dimensional dissipation, along the first (u-) direction.

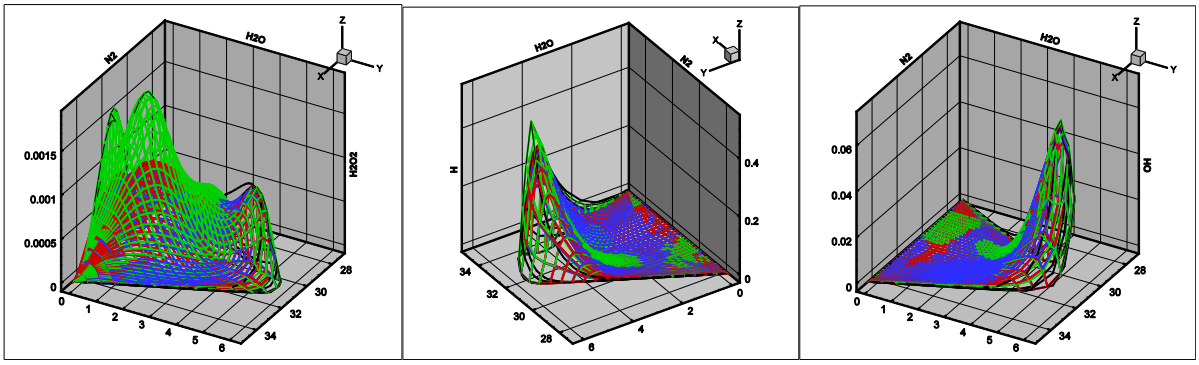

Fig. 4. REDIMs in projection to some species mole numbers. The red mesh shows the REDIM where the transport in both directions u and v was accounted for, blue mesh – only u, green mesh – only v. The black curves are stationary solutions for different scalar dissipation rates.

4 Conclusions

The mutual alignment of the local diffusion fluxes of different state variables (temperature and species) in a non-premixed turbulent combustion scenario is studied using 3D DNS data. In the considered flame configuration, the diffusion fluxes of different species display considerable directional scatter, while residing approximately within a two-dimensional subspace of 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 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 difference, while noticeable, was quite small. We conclude that, for the conditions studied in the DNS on hand, the two-dimensional dissipative transport is of negligible influence on the overall behavior of the reaction-diffusion system. It is possible, however, that for stronger turbulence or when more detailed models for dissipative transport are used, the multi-dimensional transport gains importance as an influencing factor. This is subject of future work, employing the same methodology as presented in this paper.

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