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A DNS-based study on the gradient estimates for the Reaction-Diffusion Manifold (REDIM) model

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Abstract

The REDIM approach for reduced modelling of combustion systems allows to specify a so-called gradient estimate, which specifies the interaction between dissipative transport and chemical reaction. To obtain information about the gradients occurring in a typical combustion scenario, DNS data from a turbulent flame which were computed using detailed chemistry were studied. A method is developed which maps the gradient vectors from the DNS data to a form that is directly usable as gradient estimate for the REDIM method. A REDIM is then computed using the DNS-based gradient estimate, and the reduced state space formed by the REDIM method is compared to the DNS data.

1   Introduction

The construction of reliable reduced models for the efficient simulation of combustion processes which are governed by strongly coupled thermo-chemical and advection/diffusion processes (e.g. regimes of combustion of lean mixtures with instabilities, re-ignition, local extinction etc.) is a challenging task [1, 2]. For these systems, the influence of molecular diffusion and advection (via the bulk flow of a reacting gas/fluid) strongly competes with chemical reaction, complicating extremely most of known concepts of model reduction (see e.g. [3, 4]).The crucial reactive-diffusive aspect of combustion systems can be accounted for by the concept of Reaction-Diffusion Manifolds (REDIM, [5]). Similar to other manifold-based methods (like ILDM [6], flamelets or flamelet-generated manifolds (FGM) [7, 8]), the system dynamics is approximated by a few (typically, one or two) variables, the so-called reduced variables. The REDIM method requires an estimation of the spatial gradients of the reduced variables as a function of those reduced variables. This is needed to characterize the diffusive transport in the reacting system and its coupling with chemical reactions.

In this paper, the role of the species gradients in the REDIM concept is discussed. Perspectives of using the results of DNS data analysis for the flame structure characterization are outlined. It is shown how the DNS data of a turbulent flame can be used to obtain information on the species gradients occurring in a typical combustion scenario. A scheme to identify location, orientation and directedness of the reaction zone is used to map the gradient vectors from the DNS to a form that can directly be used as an input to the REDIM method.

2   Approach

In order to show how the coupling can be treated and the influence of transport properties can be accounted for in the reduced model, the original system of equations governing the reacting flow can be cast as following [9]

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

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 $\psi_i = w_i / M_i, i = 1,...,n_s$ (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 is then defined as $M = \{\psi = \psi(\theta), \quad \theta = (\theta_1,...,\theta_m)\}, m << n$.

The REDIM methods is based on the solution of the REDIM equation [5, 10] following from the invariance relations (see e.g. [11]) as

$$\begin{cases} \dfrac{\partial \psi(\theta,\tau)}{\partial \tau} = (I - \psi_\theta \psi_\theta^+) \cdot \left[F(\psi(\theta)) + \dfrac{1}{\rho} \text{div}(D(\psi(\theta))\psi_\theta(\theta)\text{grad}\,\theta) \right] \\ \psi(\theta,0) = \psi_0(\theta) \end{cases} \qquad (2)$$

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

$$\text{grad}\,\psi(\theta) = \psi_\theta(\theta)\text{grad}\,\theta \qquad (3)$$

Hence, information on the gradients and their dependence on the reduced variable θ must be specified before the stationary solution of Eq. (2) can be calculated. Because the reduced state space of a reacting system is defined by mainly two processes (reaction and diffusion [10], see Eq. (2)), an appropriate methodology of the gradients estimations has to incorporate consistently both these processes such that the final reduced space (manifold) will describe the system states in consistence with the problem's boundary and initial conditions. To obtain a gradient estimate, DNS data from a non-premixed, slightly turbulent flame are studied. The following strategy is suggested. First, the flame structure of the 2D DNS data is considered, analyzed and species' gradient estimations are extracted. Then these gradients are employed in the REDIM equation (solution of Eq. (2)) and, finally, the resulting REDIM-based reduced space is compared with the original DNS flame data.

Data from a 2D-DNS of a non-premixed turbulent flame situated in a counter-flow of air and a diluted N_2/H_2 (75%/25% by mole) mixture at atmospheric pressure and T=298K are studied. The DNS features detailed hydrogen/air chemistry, and a simplified transport model with a Lewis-number 1 assumption. Simulations were set up for a two-dimensional quadratic spatial domain with a side length of 1 cm, with a spatial grid spacing of 20 micrometer in each direction. The DNS was initialized with profiles from a laminar, one-dimensional non-premixed H_2/N_2-air flame, which were extended to two-dimensional space. A field of synthetic turbulence was imposed with a turbulent kinetic energy distribution given by a von Karman relation with Pao correction. The code parcomb [12] was used to conduct the DNS calculations, integrating the system of Navier-Stokes equations of the underlying combustion system. The DNS deliver the spatio-temporal evolution of the system, i.e., at each point in the computational domain, the full state vector ψ at any time and spatial location, $\psi(t,x,y)$ in Eq. (1), is available.

3   Results and Discussion (DNS data analysis, REDIM construction)

From the DNS, auxiliary data were inferred in post-processing steps, namely gradients of scalars and the chemical rate of entropy production, which is crucial for the following consideration. The DNS results were analyzed to infer the magnitude and relative orientation of gradients of the reduced variables in a turbulent combustion scenario. Calculating the entropy production rate due to chemical reaction, $\dot{s}_{chem} = Q$ allowed to identify regions of chemical activity. This region forms a wave-like structure, which is folded and corrugated by the turbulent flow field, and sometimes appears to be interrupted (as exemplified by Fig.1, middle).
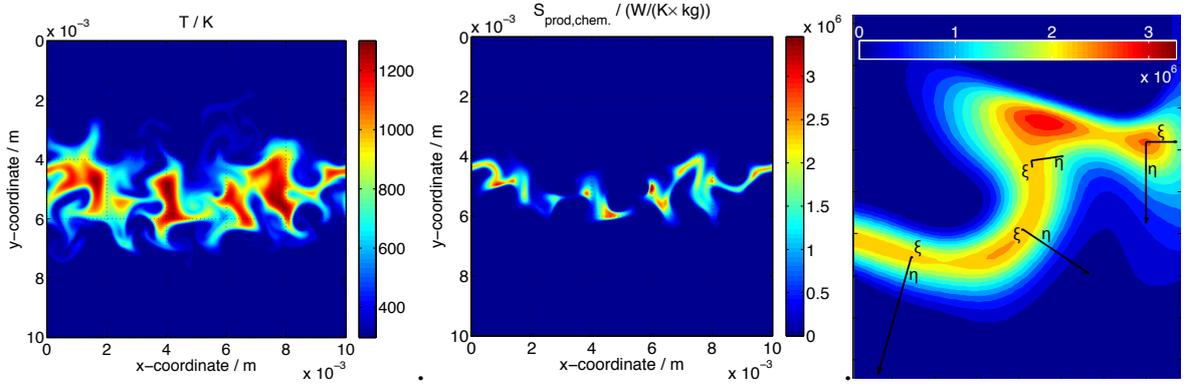
Fig. 1. Left: Typical instantaneous temperature field (in K) of the DNS. Middle: Specific entropy production Q (in W/(kg·K)) by chemical reaction, marking zones of chemical activity. Right: Principal directions at several sample points along the reaction zone (shown by vectors ξ and η). The two leftmost points are situated in regions with clear separation of the magnitude of principal curvatures (norm of vector ξ is much smaller than the norm of η); for the two rightmost points, the norms are comparable.

The reaction zone often exhibits a quasi-one dimensional, filamentary structure, but can also be bulky and essentially two-dimensional.

To characterize the change of scalars along the reaction zone and perpendicular to it, it is advantageous to introduce a local coordinate system which is aligned to the reaction zone. Such coordinates can be introduced in several ways, e.g., based on iso-contour lines of scalars (like the mixture fraction in the non-premixed flame model). Here, we use the directions of principal curvature of the entropy production field Q(x,y). This can be accomplished by forming the local Hessian $H = \left[\partial^2 Q / \partial x_i \partial x_j \right]$ (i=1,2).

The matrix H is a 2x2 symmetric matrix (the two mixed second derivatives are identical) and can therefore be decomposed according to $H = V \Lambda V^{-1}$, with a diagonal matrix Λ and an orthonormal matrix V, where both V and Λ have real coefficients. The eigenvector in V corresponding to the eigenvalue with smallest magnitude yields the spatial direction along which Q(x,y) has smallest curvature. This eigenvector v_{min}, multiplied with the corresponding eigenvalue λ_{min}, is shown for several points along the reaction zone as vector ξ in Fig. 1, on the right side: ξ = $\lambda_{min} \cdot v_{min}$. The vector v_{max} corresponding to the eigenvalue λ_{max} with largest magnitude points into the direction of largest curvature (vectors η=$\lambda_{max} \cdot v_{max}$ in Fig. 1, right side).

The local coordinate system defined by v_{min} and v_{max} affords a similar functionality in identifying the location and orientation of the reaction zone like, e.g., the coordinate system spanned by tangential and normal vectors to iso-contour lines of mixture fraction in the non-premixed flamelet model. The v_{min}-v_{max} system, however, is generic with respect to the kind of combustion system (is the same for fully-, partially- or non-premixed combustion systems). This local coordinate system is used to obtain gradient estimates for use in the REDIM approach. A measure of the strength of the gradient of some scalar ψ within the reaction zone is inferred by using the component of the gradient vector of ψ_i in v_{max} (η) – direction, i.e., in the direction that is normal to the main orientation of the reaction front. This component grad(ψ_i)$^{\parallel}$ can be computed from the projection of grad(ψ_i) onto v_{max} according to

$$\text{grad } \psi_i^{\parallel} = v_{max}^T \left(v_{max} v_{max}^T \right) \text{grad} \psi_i \qquad (4)$$

The individual components of grad(ψ_i)$^{\parallel}$ (i=1,…,n) in turn can be assembled into a new vector, which is used as the gradient estimate grad(ψ) (cf. section 2) in the REDIM approach, finally resulting in the gradient estimate for the reduced variables from Eq. (3), grad(θ). After extracting the gradients from a large number of DNS points, information about the shape of grad(θ) as a function of θ for a turbulent combustion scenario is obtained. These functions, obtained from a regression through a large set of DNS data points, are shown in Fig. 2, left.
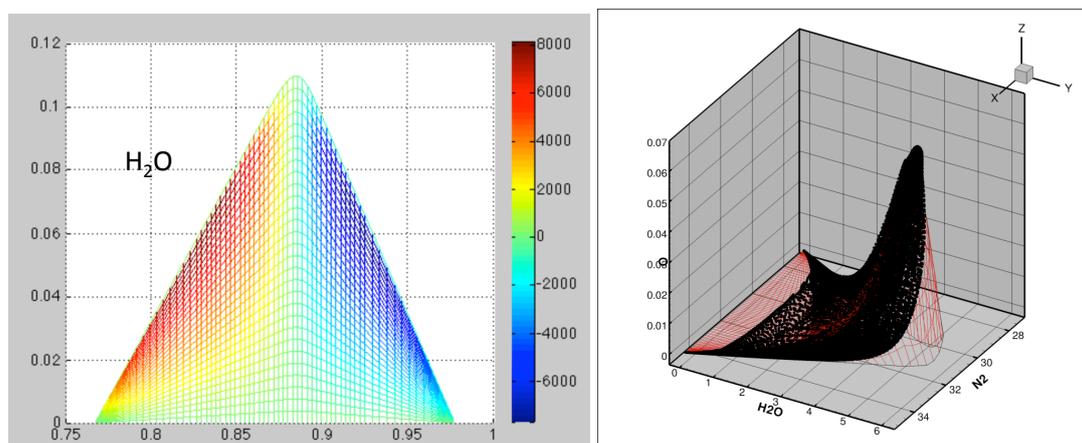
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Fig. 2. Left: DNS-based gradient estimates grad(ψ_i) as a function of θ, shown here for H_2O. The x- and y-axes in the diagrams are mass fraction of N_2 and H_2O, respectively, and the colors represent the gradient estimate in units of specific mole numbers/m. Right: Comparison of the correlation between N_2, H_2O and O specific mole numbers predicted by 2D REDIM (red surface, computed using a gradient estimation from the DNS data), and the DNS data (black symbols).

Using the gradients extracted from the DNS, a REDIM was computed. This REDIM describes a two-dimensional surface in state space spanned by the components of ψ. The position of this surface can be compared to the state space location of the DNS which were used to supply the gradient estimate underlying the REDIM. The DNS data points are mostly very close to the REDIM surface, even when radicals like OH or O are considered (Fig. 2, right).

4   Conclusions

DNS data were used to provide a gradient estimate for the REDIM model. The estimates are obtained from the DNS using a novel generic approach to identify the reaction zone in the DNS data, as well as its local properties (e.g., orientation and alignment relative to iso-lines of scalar fields). The REDIM resulting from these gradient estimates then describes the correlations of DNS data in state space quite well. Future work will focus on using this REDIM to provide a reduced model for the chemical source terms, which is then employed for another reduced DNS calculation, which can be directly compared to DNS results obtained using fully detailed chemical kinetics.

5   Acknowledgments

6   References

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