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Principal component transport in turbulent combustion: *A posteriori* analysis

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ABSTRACT

This paper presents *a posteriori* validation of the solution of a turbulent combustion problem based on the transport of principal components (PCs). The PCs are derived from *a priori* principal component analysis (PCA) of the same composition space. This analysis is used to construct and tabulate the PCs' chemical source terms and diffusion coefficients in terms of the PCs using artificial neural networks (ANN). The *a posteriori* validation is implemented on a stand-alone one-dimensional turbulence (ODT) simulation of Sandia Flame F resulting in a very good reconstruction of the original thermo-chemical scalars profiles with 3 PCs at different downstream distances.

1. Introduction

Principal component analysis (PCA) has been proposed as a method to reduce the composition space of combustion systems [1–13]. The different studies in Refs. [1–13] have adopted different strategies to reduce the composition space and explore the use of PCA. The construction of PCs requires a computational/experimental database that is available *a priori*. The database must emulate the composition space of interest either through the generation of a representative problem (with all its dimensional complexity) or a simplified problem (as adopted here). Such a strategy is not new. For example in the steady flamelet approach, flamelet libraries may be generated using 1D simulations of strained flames.

Because there is no preset number or type of PCs, PCA can potentially be used to reduce composition spaces where obvious variables to parameterize them are not known *a priori*. This may include problems with mixed modes (e.g. premixed, non-premixed and partially premixed), regimes (e.g. flamelet, distributed reaction) or where transient and non-equilibrium effects are present (e.g. extinction and re-ignition, autoignition). Addressing the type of database to be used remains a challenging problem that requires further study. Nonetheless, PCA can provide a robust tool to produce generalized flame libraries for less accessible problems.

In the last decade or so, different uses for PCA have been proposed. The first approach is related primarily to the generation of a reduced description of computational or experimental databases, such as the studies in Refs. [1,2]. However, since the work of Sutherland and Parente [3], there was increased emphasis on the solution of combustion problems through primarily two competing strategies. The first one is based on the transport of principal components [3,10,12–14], which involves the solution of transport equations for the principal components instead of the transport of the vector of thermo-chemical scalars (e.g. energy, composition). Sutherland and Parente [3] presented a governing equation for the PCs and derived expressions for the PCs source terms and diffusion fluxes. In linear PCA, such expressions are relatively trivial and relate linearly the PCs source and diffusive flux terms to the thermo-chemical scalars source and diffusive flux terms.

More recently, the authors have proposed an alternative tabulation of the PCs in terms of the thermo-chemical scalars and *vice versa* using artificial neural networks [10,12–14]. In a more recent study [14], we demonstrated that tabulation represents a better strategy than matrix inversion from a reduced set of PCs to the original thermo-chemical scalars vector. More importantly, we proposed expressions for the diffusion coefficients of the PCs in terms of the thermo-chemical scalars diffusion coefficients [13]. The derivation represents another important breakthrough toward the solution of PCs transport equations as it offers a method to tabulate diffusion coefficients, which are properties of the PCs.

The second approach adopted by other authors is to identify a reduced set of the original thermo-chemical scalars using PCA; this set can be used to represent all the thermo-chemical scalars [9,11]. As an additional "chemistry reduction" method, the use of "representative scalars" can potentially decrease significantly the computational cost of combustion simulation.

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In the present work, we adopt the first approach. The objective of this study is to validate the approach of transporting principal components (PCs) using a canonical turbulent flame problem, the Sandia Flame F and PCA. Addressing a problem with sufficiently complex composition space provides useful validation for the proposed approach. To our knowledge, this work is the first implementation of PCs transport within the content of a turbulent combustion problem and represents a natural extension of previous studies by the authors to develop optimum strategies for the construction of principal components using linear and non-linear methods and key transport terms necessary for the transport of PCs.

In the following, we discuss the main steps to carry out the transport of principal components (Section 2). Then, results of these solutions are compared to those corresponding to the transport of thermo-chemical scalars (Section 3). Finally, some concluding remarks are made (Section 4).

2. Procedure for *a posteriori* validation

The PCA analysis starts with detailed experimental and computational data of thermo-chemical scalars' vectors defined at different data points (e.g. different times or positions in space), such as what is adopted here based on temperature and composition $\boldsymbol{\theta} = (T, Y_1, \ldots, Y_{N-1})^{\mathrm{T}}$ where T is the mixture temperature and the mass fractions of $N-1$ species in the mixture are denoted by $Y_1, Y_2, \ldots, Y_{N-1}$ all defined at a given data point; however, it is more convenient to use a detailed simulation data, e.g. direct numerical simulation (DNS), such that reaction rates and transport properties for all relevant scalars can be determined. PCA analysis results in a vector of principal components: $\boldsymbol{\Psi} = (\Psi_1, \Psi_2, \ldots, \Psi_N)^{\mathrm{T}}$ where the Ψ's are the principal components (PCs).

In linear PCA, a simple expression relates the principal components to the original thermo-chemical scalars vector or a subset of that vector [3]:

$$\boldsymbol{\Psi} = \mathbf{Q}^{\mathrm{T}}\boldsymbol{\theta} \tag{1}$$

The $N \times N$ matrix of orthonormal eigenvectors, $\mathbf{Q}$, of the correlation matrix (columns), $\mathbf{C}$, is constructed from data based on m temporal and spatial realizations of $\boldsymbol{\theta}$. This data may be based on a canonical problem that reproduces important features in composition space of the desired problem.

The relation in (1) can be truncated such that only the N_{PC} higher eigenvalues are retained resulting in a more manageable representation of the data, where $N_{\mathrm{PC}} < N$. We expect N_{PC} to be much smaller than N for the reduction process to be practical. Evidence that an aggressive truncation is possible can be found in Refs. [2,3,10]. An $N \times N_{\mathrm{PC}}$ matrix $\mathbf{A}$ may be constructed, which contains only the first N_{PC} leading eigenvectors of matrix $\mathbf{Q}$ based on the choice of the number of eigenvectors retained [3]:

$$\boldsymbol{\Psi}^{\mathrm{red}} = \mathbf{A}^{\mathrm{T}}\boldsymbol{\theta}. \tag{2}$$

Here $\mathbf{A}$ corresponds to the matrix made up of the leading N_{PC} eigenvectors of $\mathbf{Q}$. The superscript "red" corresponds to the selected reduced set of PCs chosen to represent the data. If a single linear PCA is adopted for the entire data, the matrices $\mathbf{Q}$ and $\mathbf{A}$ are constant matrices.

To be able to solve transport equations for the PCs, we must be able to derive these transport equations and evaluate their key transport terms. The original thermo-chemical scalars are subject to a set of transport equations of the general form [3]:

$$\rho\frac{D\boldsymbol{\theta}}{Dt} = \nabla\cdot\mathbf{J}_{\boldsymbol{\theta}} + \mathbf{S}_{\boldsymbol{\theta}} \tag{3}$$

where $\mathbf{J}_{\boldsymbol{\theta}}$ and $\mathbf{S}_{\boldsymbol{\theta}}$ correspond to the diffusive fluxes and the chemical source terms for the original thermo-chemical scalars' vector, $\boldsymbol{\theta}$, respectively. Sutherland and Parente [3] proposed a similar form for the PCs' transport equations [3,13]:

$$\rho\frac{D\boldsymbol{\psi}}{Dt} = \nabla\cdot\mathbf{J}_{\boldsymbol{\psi}} + \mathbf{S}_{\boldsymbol{\psi}} \tag{4}$$

where $\mathbf{J}_{\boldsymbol{\psi}}$ and $\mathbf{S}_{\boldsymbol{\psi}}$ correspond to the diffusive fluxes and the chemical source terms for the PCs, respectively.

The simple linear relation between PCs and the thermo-chemical scalars vector enabled Sutherland and Parente [3] to derive expressions for $\mathbf{J}_{\boldsymbol{\psi}}$ and $\mathbf{S}_{\boldsymbol{\psi}}$: $\mathbf{S}_{\boldsymbol{\psi}} = \mathbf{Q}^{\mathrm{T}}\mathbf{S}_{\boldsymbol{\theta}}$ (or $\mathbf{S}_{\boldsymbol{\psi}}^{\mathrm{red}} = \mathbf{A}^{\mathrm{T}}\mathbf{S}_{\boldsymbol{\theta}}$) and $\mathbf{J}_{\boldsymbol{\psi}} = \mathbf{Q}^{\mathrm{T}}\mathbf{J}_{\boldsymbol{\theta}}$ (or $\mathbf{J}_{\boldsymbol{\psi}}^{\mathrm{red}} = \mathbf{A}^{\mathrm{T}}\mathbf{J}_{\boldsymbol{\theta}}$).

To proceed further in evaluating the transport terms for the PCs, we have adopted a simplified form for the diffusive flux assuming that a set of diffusion coefficients can be constructed for the principal components [13]:

$$\mathbf{J}_{\boldsymbol{\psi}} = \rho\mathbf{D}_{\boldsymbol{\psi}}\nabla\boldsymbol{\psi} \tag{5}$$

where $\mathbf{D}_{\boldsymbol{\Psi}}$ is the matrix of diffusion coefficients for the PCs. Based on that form, we have derived an expression for $\mathbf{D}_{\boldsymbol{\Psi}}$ in terms of the matrix of diffusion coefficients for the thermo-chemical scalars, $\mathbf{D}_{\boldsymbol{\theta}}$, as follows [13]:

$$\mathbf{D}_{\boldsymbol{\psi}} = \mathbf{Q}^{\mathrm{T}}\mathbf{D}_{\boldsymbol{\theta}}\mathbf{Q}. \tag{6}$$

This expression provides a direct method for determining the diffusion coefficient of the PCs, as a "property" of the PCs, given the diffusion coefficients of the thermo-chemical scalars. A similar expression was derived for non-linear PCA methods [12]; however, the matrix $\mathbf{Q}$, for these methods, are interpreted as a Jacobian relating variations in $\boldsymbol{\theta}$ to variations in $\boldsymbol{\Psi}$. As indicated in Ref. [13], the characteristics of the matrix $\mathbf{D}_{\boldsymbol{\Psi}}$ are not as convenient as those of $\mathbf{D}_{\boldsymbol{\theta}}$. First, while $\mathbf{D}_{\boldsymbol{\theta}}$ is a diagonal matrix, we expect $\mathbf{D}_{\boldsymbol{\Psi}}$ to be a full matrix; although, for linear PCA, and because of the properties of matrix $\mathbf{Q}$, we expect $\mathbf{D}_{\boldsymbol{\Psi}}$ to be a symmetric matrix. More importantly, there is no guarantee that the coefficients of $\mathbf{D}_{\boldsymbol{\Psi}}$ are positive; and their sign depends on the contributions of the components of $\mathbf{Q}$. Therefore, $\mathbf{D}_{\boldsymbol{\Psi}}$ may fulfill some of the characteristics that make it, mathematically, a matrix of binary diffusion coefficients. However, the possibility that these coefficients may be negative does degrade their physical meaning. More importantly, these negative coefficients correspond to a mechanism for counter-gradient diffusion, a potential source for numerical instability, if not addressed properly during the numerical integration. In the present study, we propose a linear transformation of the retained PCs to maintain a dominance of the diagonal terms and reduce the magnitude of negative diffusion coefficients.

Based on the above discussion, the solution of PCs' transport equations must be preceded by the following steps:

1. *Generation of the database:* A numerical database is generated. In the present validation study, this is achieved using stand-alone one-dimensional turbulence (ODT) simulations of the Sandia Flame F.
2. *PCA analysis:* A subset of the thermo-chemical scalar vector is selected on which PCA is implemented [10]. PCA is implemented to determine the PCs. Preliminary analysis is carried out to determine the number of PCs to be retained.
3. *Tabulation:* Reaction source terms and diffusion coefficients for the PCs are tabulated as functions of the principal components. For the reconstruction of the thermo-chemical scalars' vector, this vector is also tabulated as a function of the PCs vector. Instead of an inversion relation, tabulation using ANN is implemented [10,12–14]. Initialization of the problem also requires that the PCs are tabulated based on the full set of thermo-chemical scalars. As outlined below, tabulation of the viscosity and the mixture density as functions of the PCs is also implemented.