

Systematic Definition of Progress Variables and Intrinsically Low-Dimensional, Flamelet Generated Manifolds for Chemistry Tabulation

A. Najafi-Yazdi^{a,*}, B. Cuenot^b, L. Mongeau^a

^a*Department of Mechanical Engineering, McGill University, Montreal, QC, H3A2K6, Canada*

^b*CERFACS, CFD Team, 42 Avenue G. Coriolis, 31057 Toulouse Cedex 01, France*

Abstract

A systematic method to define progress variables for chemistry tabulation is presented. The method is mathematically based on the Principal Component Analysis (PCA) of the mass fraction of species in the composition space. The present approach is analogous to eigenvalue analysis of Intrinsic Low Dimensional Manifolds. Thus, the present study provides a similar strong mathematical formulation for flamelet-based tabulation methods. Moreover, the new method is designed to provide the minimum number of linearly independent progress variables, for a user-prescribed desirable accuracy, in representing the thermo-chemical states of interest. Hence, it is suggested that the flamelet-based tabulations created with the new approach be called *Intrinsically Low-Dimensional, Flamelet Generated Manifolds* (IL-FGM).

Keywords: Chemistry Tabulation, Flamelet Methods, Flamelet Generated Manifold, Turbulent Combustion

1. Introduction

Numerical simulations of turbulent reacting flows with a full description of complex chemistry remain prohibitively expensive due to computational

*Corresponding author.

Address: Room 270, Macdonald Engineering Building, 817 Sherbrooke Street West, Montreal, H3A 2K6, QC, Canada. Fax: 514-398-7365

Email address: alireza.najafiyazdi@mail.mcgill.ca (A. Najafi-Yazdi)

resources limitations. Several methods have been proposed to address this problem. These approaches include reducing the chemical scheme in intrinsic low dimensional manifolds(ILDM) [1, 2], or using flamelet-based approaches such as the flamelet-progress variable (FPV) [3], flame prolongation of ILDM (FPI) [4], and flamelet generated manifolds (FGM) [5].

The basic idea of the ILDM method is to describe the complex chemistry with an attracting, low dimensional, manifold in the composition space. This manifold is identified through an eigenvalue analysis of the chemical scheme. Although ILDM method has a strong mathematical foundation, its accuracy deteriorates in low temperature regions. This is due to the fact that the transport of species through convection and diffusion is neglected in the ILDM formulation, while these phenomena become important in the dynamics of low temperature regions.

To overcome this limitation, flamelet-based approaches use the numerical solution of one-dimensional premixed flames or nonpremixed flamelet equations to construct the look-up tables which describe the chemistry. In these methods, the thermo-chemical states of interest are calculated and tabulated, prior to the simulation, as functions of a set of independent variables, referred to as progress variables.

The flamelet table can be mathematically represented as

$$\Psi = F(c_1, c_2, \dots, c_n) = F(\mathbf{c}), \quad (1)$$

where Ψ denotes the vector of all thermo-chemical properties of interest, and \mathbf{c} represents the vector of progress variables. The progress variables should be defined such that all thermo-chemical states of interest can be uniquely identified. Moreover, it is desirable to keep the number of progress variables, and hence, the table dimensions at minimum to avoid prohibitive memory requirements.

So far, the definition of progress variables has been somewhat arbitrary which results in a weaker mathematical foundation for FPI and FGM methods [6]. The progress variable has been conventionally defined using the mass fraction of major species such as CO_2 , CO , and H_2O . However, such definitions usually lead to inaccurate results for rich mixtures, or heavy hydrocarbon fuels as they decompose before significant heat release. The ambiguity in defining progress variables can become problematic as the number of progress variables in a tabulation increases. Ad-hoc progress variables might not necessarily be linearly independent to form an orthogonal base in

the composition space. This can result in loss of accuracy in identifying a specific thermo-chemical state in the tabulation.

In this paper, we propose a systematic method to define the progress variables for FGM and FPI. The method is mathematically based on the Principal Component Analysis (PCA) of the composition space, which is itself constructed from one-dimensional flame simulations. Also known as Proper Orthogonal Decomposition (POD), the Karhunen-Loeé Decomposition, and the Hotelling transform, PCA is widely used for reduced-order modeling, low-dimensional representations of phenomena, and data reduction [7]. The application of PCA in the present study is analogous to the eigenvalue analysis of ILDM, providing FGM and FPI with a similar strong mathematical formulation.

Using PCA, the proposed approach is designed to provide the minimum number of linearly independent progress variables in representing the thermo-chemical states of interest. Hence, it is suggested that the flamelet-based tabulations created with the new approach be called *Intrinsically Low-Dimensional, Flamelet Generated Manifolds* (IL-FGM).

The present paper is organized as follows. Some background on the Principal Component Analysis and the Singular Value Decomposition (SVD) is reviewed in Sec. 2. The new approach to define progress variable and constructing IL-FGMs are presented in Sec. 3. Some numerical examples are provided in Sec. 4. Conclusions are drawn in Sec. 5

2. Principal Component Analysis

2.1. Background

Consider a set of n measurements of a physical phenomenon. Each measurement yields a set of m variables which describe the physical state of the system and can be represented by a $m \times 1$ vector \mathbf{x} . In the present study, the vector \mathbf{x} consists of the mass fraction of all species involved in the given chemical mechanism,

$$\mathbf{x} = [Y_1 \quad Y_2 \quad \cdots \quad Y_m]^T, \quad (2)$$

where Y_i represents the mass fraction of the species i , and m is the number of species in the mechanism. The data obtained from the n measurements can be represented by a $m \times n$ matrix,

$$\mathbf{X} = [\mathbf{x}_1 \quad \mathbf{x}_2 \quad \cdots \quad \mathbf{x}_n]. \quad (3)$$

Each measurement, \mathbf{x}_i , denotes a point in the m -dimensional composition space. The matrix \mathbf{X} represents a cloud of point on a manifold which specifies different states of the system.

The goal of PCA is to find the optimal linear combination of original bases to minimize the redundancy, and represent data set with a reduced number of dimensions. Hence, PCA tries to achieve this goal by finding the principal directions in the data set, along which maximum variations of data is expected.

2.2. Identification of the principal directions

Let \mathbf{X} and \mathbf{C} be $m \times n$ matrices of the original data set, and its projection along the principal directions, respectively. The goal is to find an $m \times m$ -transformation matrix \mathbf{W} that relates \mathbf{X} and \mathbf{C} through the following relation:

$$\mathbf{C} = \mathbf{W} \mathbf{X}. \quad (4)$$

Each component of \mathbf{C} is a dot-product of vector \mathbf{x}_i with the corresponding row of \mathbf{W} . In other words, the matrix \mathbf{C} is the projection of the original data set \mathbf{X} on the new basis defined by row of \mathbf{W} (i.e. \mathbf{w}_i 's). It should be noted that PCA requires that \mathbf{w}_i vectors be orthonormal.

To have the optimal representation of the original data set, it is expected that \mathbf{C} have minimum redundancy, and the new bases be linearly independent from each other. This is achieved by defining \mathbf{W} such that the covariance matrix,

$$\mathcal{C}_{\mathbf{C}} = \frac{1}{n} \mathbf{C} \mathbf{C}^T, \quad (5)$$

is diagonal. The covariance matrix of the transformed data set, $\mathcal{C}_{\mathbf{C}}$, can be written in terms of the covariance matrix of the original data set, $\mathcal{C}_{\mathbf{X}}$, as follows:

$$\begin{aligned} \mathcal{C}_{\mathbf{C}} &= \frac{1}{n} \mathbf{C} \mathbf{C}^T \\ &= \frac{1}{n} (\mathbf{W} \mathbf{X}) (\mathbf{W} \mathbf{X})^T \\ &= \mathbf{W} \left(\frac{1}{n} \mathbf{X} \mathbf{X}^T \right) \mathbf{W}^T \\ &= \mathbf{W} \mathcal{C}_{\mathbf{X}} \mathbf{W}^T. \end{aligned} \quad (6)$$

This form will be used later in Sec. 2.3 to find the matrix \mathbf{W} through the Singular Value Decomposition.

2.3. Singular Value Decomposition and Principal Component Analysis

A Singular Value Decomposition (SVD) of a $m \times n$ matrix \mathbf{X} is defined as [8]:

$$\mathbf{X} = \mathbf{U}\mathbf{S}\mathbf{V}^T, \quad (7)$$

where \mathbf{U} and \mathbf{V} are $m \times m$ and $n \times n$ orthonormal matrices, respectively. The matrix \mathbf{S} is an $m \times n$ matrix with all elements equal to zero except on the diagonal. The diagonal elements of \mathbf{S} are called the singular values of \mathbf{X} , and are in descending order. The covariance matrix of \mathbf{X} can then be expanded to yield

$$\begin{aligned} \mathcal{C}_{\mathbf{X}} &= \frac{1}{n}\mathbf{X}\mathbf{X}^T \\ &= \frac{1}{n}(\mathbf{U}\mathbf{S}\mathbf{V}^T)(\mathbf{U}\mathbf{S}\mathbf{V}^T)^T \\ &= \frac{1}{n}\mathbf{U}\mathbf{S}\mathbf{V}^T\mathbf{V}\mathbf{S}^T\mathbf{U}^T \\ &= \frac{1}{n}\mathbf{U}\mathbf{S}\mathbf{S}^T\mathbf{U}^T. \end{aligned} \quad (8)$$

Equation (8) can be further simplified to give

$$\mathbf{U}^T\mathcal{C}_{\mathbf{X}}\mathbf{U} = \frac{1}{n}\mathbf{S}\mathbf{S}^T, \quad (9)$$

which reveals that $\mathbf{U}^T\mathcal{C}_{\mathbf{X}}\mathbf{U}$ is a diagonal matrix. If \mathbf{W} is chosen to be \mathbf{U}^T , eq. (6) and (9) can be combined to yield

$$\mathcal{C}_{\mathbf{C}} = \mathbf{W}\mathcal{C}_{\mathbf{X}}\mathbf{W}^T = \mathbf{U}^T\mathcal{C}_{\mathbf{X}}\mathbf{U} = \frac{1}{n}\mathbf{S}\mathbf{S}^T. \quad (10)$$

Since $\mathcal{C}_{\mathbf{C}} = \frac{1}{n}\mathbf{S}\mathbf{S}^T$ is diagonal, it is concluded that columns of \mathbf{U} are the principal components of the data set \mathbf{X} .

Another important property of the SVD is that

$$\tilde{\mathbf{X}}_{m \times n}^k = \mathbf{U}_{m \times k}\mathbf{S}_{k \times k}\mathbf{V}_{n \times k}^T \quad k < \min(m, n), \quad (11)$$

is the closest approximation of \mathbf{X} in the least square sense for a k -dimensional subspace. The matrix $\tilde{\mathbf{X}}^k$ is commonly referred to as the approximation of rank k to \mathbf{X} . Matrices $\mathbf{U}_{m \times k}$, and $\mathbf{V}_{n \times k}$ are formed from the first k columns of $\mathbf{U}_{m \times m}$ and $\mathbf{V}_{n \times n}$, respectively; similarly, the matrix $\mathbf{S}_{k \times k}$ is a diagonal matrix made from the first k singular values of \mathbf{X} .

Therefore, SVD provides not only just a new set of basis to represent the data, but also the best set of base vectors to approximate a given data set with the fewest possible dimensions.

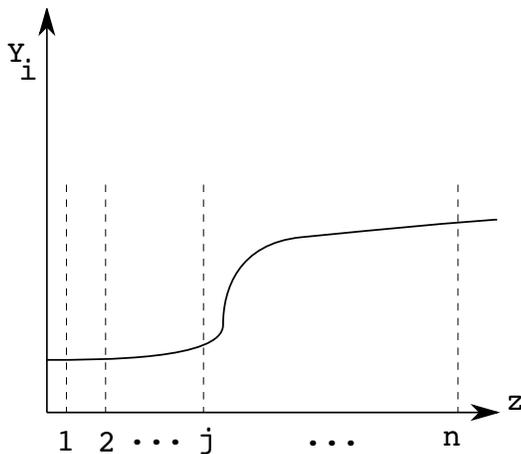


Figure 1: A schematic profile of the mass fraction of a species in a one-dimensional freely propagating flame. The flame is sampled at n stations in the physical domain to construct the data set.

3. Systematic Definition of Progress Variables, and Intrinsically Low-Dimensional, Flamelet Generated Manifolds

Consider the numerical solution of a freely propagating flame as illustrated in Fig. 1. Such solutions are tabulated in FGM and FPI. Considering a chemical mechanism with m species, the one-dimensional flame is sampled at n stations to form a $m \times n$ data set in the form of matrix \mathbf{X}^1 , which represents the flamelet manifold in the composition space \mathbb{R}^m .

Rather than using an ad-hoc definition, it is suggested that progress variables be defined as linear combinations of species mass fractions,

$$c_i = \sum_{j=1}^m w_{ij} Y_j, \quad (12)$$

such that they form the principal directions of the flamelet manifold in the composition space. As discussed in Sec. 2, the principal directions yield the best representation of a data set with minimum number of dimensions. The magnitude of the singular values of matrix \mathbf{X} indicates how important the

¹The dataset \mathbf{X} can also include samples from simulations with variable equivalence ratio, inlet temperature, or strain rate depending on the intended application.

corresponding progress variable is in the tabulation, and how many progress variables are needed. This results in a systematic way of defining the progress variables for Intrinsically Low-dimensional, Flamelet-Generated Manifolds (IL-FGM). Equation (12) can be recast in the matrix form to yield eq. (4). Thus, the weighting coefficients w_{ij} 's can be obtained from the SVD of matrix \mathbf{X} as discussed in Sec. 2.3.

4. Numerical Examples

In this section, the application of IL-FGM is demonstrated for mono-dimensional and multi-dimensional flamelets. It is important to mention that the additional cost of PCA was found to be quite small, a fraction of a second, compared to the computational time that was required to simulate each flamelet.

4.1. Flamelets with a single-progress variable

Two flamelets, each generated from the numerical solution of freely propagating flame in a CH_4 -air mixture, were considered as the first test cases. The GRI-30 mechanism [9] was used to describe the complex chemistry. The inlet condition fresh gases were set to $P = 1 [atm]$ and $T = 473 [K]$. The two flamelets were generated for equivalence ratios $\phi = 0.85$ and $\phi = 1.9$, respectively. Given the fact that each flamelet consists of the data from a single equivalence ratio calculation, it can be fully described by a single progress variable.

The weight coefficients to define the progress variable for $\phi = 0.85$ and $\phi = 1.9$, are presented in Table 1 and 2, respectively. The method automatically gives significant weight to the major reactants (O_2 , CH_4), and major products (CO_2 , H_2O). It is interesting to note that CO received a smaller weight for the fuel-lean flamelet than that for the fuel-rich one. This intrinsic ranking of important species is a significant feature of the proposed method.

To further verify that obtained progress variables can uniquely describe the flamelets, a different flame at $\phi = 0.85$ and similar inlet conditions was solved, with the computational domain length and the flame position changed. Figure 2 shows the spatial distribution of the temperature and some species mass fractions. Excellent agreement is observed between the numerical solution of the new flame with complex chemistry, and the data obtained from the previously prepared flamelet. Figure 4 compares the same results in the progress variable space.

Figure 3 shows the results of a similar test for a flame at $\phi = 1.90$. The results obtained from a flamelet, using a conventional definition of progress variable, are also shown for comparison. As it can be observed, the systematically defined progress variable yielded more accurate results than the arbitrarily defined one.

4.2. Flamelets with multi-progress variables

In many practical problems, the flamelet library may include several dimensions. For instance, the flamelet library may include solutions for various equivalence ratios and strain rates (c.f. Nguyen et al. [10]), or even two-phase flames. In such problems, the thermo-chemistry can still be tabulated in terms of several progress variables which are defined from linear combination of species mass fractions. This is demonstrated by considering a flamelet library with various equivalence ratios. It is important to note that no a-priori knowledge of chemistry or flame structure is required.

The flamelet library was obtained from the solutions of a freely propagating flame in CH_4 -air mixture at $\phi \in \{0.6, 0.7, 0.8, 0.9, 1.0, 1.1, 1.2, 1.3, 1.4, 1.5\}$. The inlet conditions for fresh gases were set to $P = 1 [atm]$ and $T = 473 [K]$.

Figure 5 shows the temperature distribution of the flamelet library as a function of the two progress variables, c_1 and c_2 . The weight coefficients for the definition of c_1 and c_2 are provided in tables 3 and 4, respectively. A Delaunay triangulation of the data set was constructed using the Computational Geometry Algorithms Library [11] for the linear interpolations.

Figure 6 shows a comparison between the numerical simulation of flame at $\phi = 1.15$ and the interpolated data from the flamelet library. Both sets of results are in excellent agreement for temperature, and major species such as CO and CO_2 . The results for minor species such as OH are not as accurate, but in overall good agreement. The results can be further improved through the use of higher order interpolations, and an increased number of flamelet solutions to expand the flamelet library.

5. Conclusion

A systematic method to define progress variables for chemistry tabulation is presented. The method is mathematically based on the the Principal Component Analysis (PCA) of the composition space. The present study provides a similar strong mathematical formulation for flamelet-based tabulation methods. Moreover, the new method provides the minimum number

of linearly independent progress variables, for a user-prescribed desirable accuracy, in representing the thermo-chemical states of interest. Hence, it is suggested that the flamelet-based tabulations created with the new approach be called *Intrinsically Low-Dimensional, Flamelet Generated Manifolds* (IL-FGM).

Some numerical examples were presented. Both mono-dimensional and multi-dimensional flamelet libraries were considered. It was demonstrated that the new method automatically identifies the species of significance importance, and takes them into account accordingly in the definition of the progress variables. Very good agreements between the flamelet-retrieved results and those obtained from the numerical simulation of freely propagating flames confirmed the effectiveness of the present approach.

The application of the present approach to simulate turbulent combustion in real combustors, with partially premixed and non-adiabatic regimes, will be studied in future works.

References

- [1] U. Maas, S. Pope, Symposium (International) on Combustion 24 (1992) 103–112.
- [2] U. Maas, S. Pope, Combustion and Flame 88 (1992) 239–264.
- [3] C. Pierce, P. Moin, Journal of Fluid Mechanics 504 (2004) 73–97.
- [4] O. Gicquel, N. Darabiha, D. Thevenin, Proceedings of the Combustion Institute 28 (2000) 1901–1908.
- [5] J. Van Oijen, L. De Goey, Combustion Science and Technology 161 (2000) 113–137.
- [6] T. Poinsot, D. Veynante, Theoretical and numerical combustion, RT Edwards, Inc., 2005.
- [7] G. Berkooz, P. Holmes, J. Lumley, Annual Review of Fluid Mechanics 25 (1993) 539–575.
- [8] G. Golub, C. Van Loan, Matrix computations, Johns Hopkins Univ Pr, 1996.

- [9] G. P. Smith, D. M. Golden, M. Frenklach, N. W. Moriarty, B. Eiteneer, M. Goldenberg, C. T. Bowman, R. K. Hanson, S. Song, J. William C. Gardiner, V. V. Lissianski, Z. Qin, GRI-30 Mechanism, 1999. Available online at http://www.me.berkeley.edu/gri_mech.
- [10] P. Nguyen, L. Vervisch, V. Subramanian, P. Domingo, *Combustion and Flame* 157 (2010) 43–61.
- [11] The CGAL Project, *CGAL User and Reference Manual*, CGAL Editorial Board, 3.7 edition, 2010. Available online at <http://www.cgal.org>.

H2	H	O	O2	OH
0.0001	0.0004	0.0060	-0.7637	0.0166
H2O	HO2	H2O2	C	CH
0.4140	-0.0002	0.0000	0.0000	0.0000
CH2	CH(S)	CH3	CH4	CO
0.0000	0.0000	0.0002	-0.1989	0.0686
CO2	HCO	CH2O	CH2OH	CH3O
0.4480	0.0000	-0.0008	0.0000	-0.0000
CH3OH	C2H	C2H2	C2H3	C2H4
-0.0002	0.0000	0.0000	0.0000	-0.0001
C2H5	C2H6	HCCO	CH2CO	HCCOH
0.0000	-0.0007	0.0000	0.0000	0.0000
N	NH	NH2	NH3	NNH
0.0000	0.0000	0.0000	0.0000	0.0000
NO	NO2	N2O	HNO	CN
0.0002	-0.0000	0.0000	0.0000	0.0000
HCN	H2CN	HCNN	HCNO	HOCN
0.0000	0.0000	0.0000	0.0000	0.0000
HNCO	NCO	N2	AR	C3H7
0.0000	0.0000	0.0106	0.0000	-0.0000
C3H8	CH2CHO	CH3CHO		
0.0000	0.0000	0.0000		

Table 1: The weight coefficients of each species, as obtained from PCA, to define the progress variable for a premixed CH_4 -air flame at $\phi = 0.85$. The results are shown up to the fourth decimal.

H2	H	O	O2	OH
0.0272	0.0000	0.0000	-0.7328	0.0001
H2O	HO2	H2O2	C	CH
0.4320	-0.0000	-0.0000	0.0000	0.0000
CH2	CH(S)	CH3	CH4	CO
0.0000	0.0000	0.0015	-0.3239	0.3706
CO2	HCO	CH2O	CH2OH	CH3O
0.3558	0.0000	-0.0006	0.0000	-0.0000
CH3OH	C2H	C2H2	C2H3	C2H4
-0.0002	0.0000	0.0395	0.0000	0.0017
C2H5	C2H6	HCCO	CH2CO	HCCOH
0.0000	-0.0004	0.0000	0.0008	0.0000
N	NH	NH2	NH3	NNH
0.0000	0.0000	0.0000	0.0000	0.0000
NO	NO2	N2O	HNO	CN
0.0000	0.0000	0.0000	0.0000	0.0000
HCN	H2CN	HCNN	HCNO	HOCN
0.0000	0.0000	0.0000	0.0000	0.0000
HNCO	NCO	N2	AR	C3H7
0.0000	0.0000	0.0067	0.0000	0.0000
C3H8	CH2CHO	CH3CHO		
0.0000	0.0000	0.0000		

Table 2: The weight coefficients of each species, as obtained from PCA, to define the progress variable for a premixed CH_4 -air flame at $\phi = 1.9$. The results are shown up to the fourth decimal.

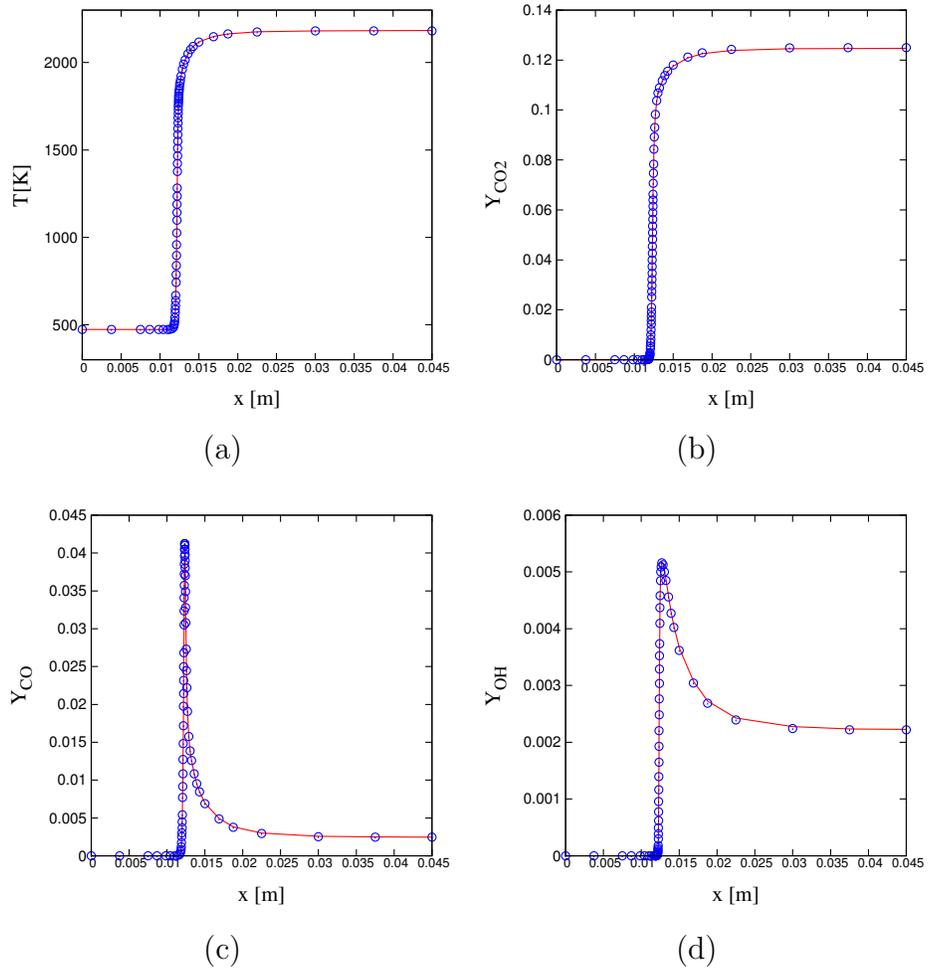


Figure 2: The structure of a freely propagating flame in CH_4 -air mixture at $\phi = 0.85$, $T_0 = 473$ [K], and $P = 1$ [atm] in the physical space; solid line: physical space solution; symbols: solution retrieved from the previously generated flamelet table. (a): temperature; (b): CO_2 mass fraction; (c): CO mass fraction; (d): OH mass fraction.

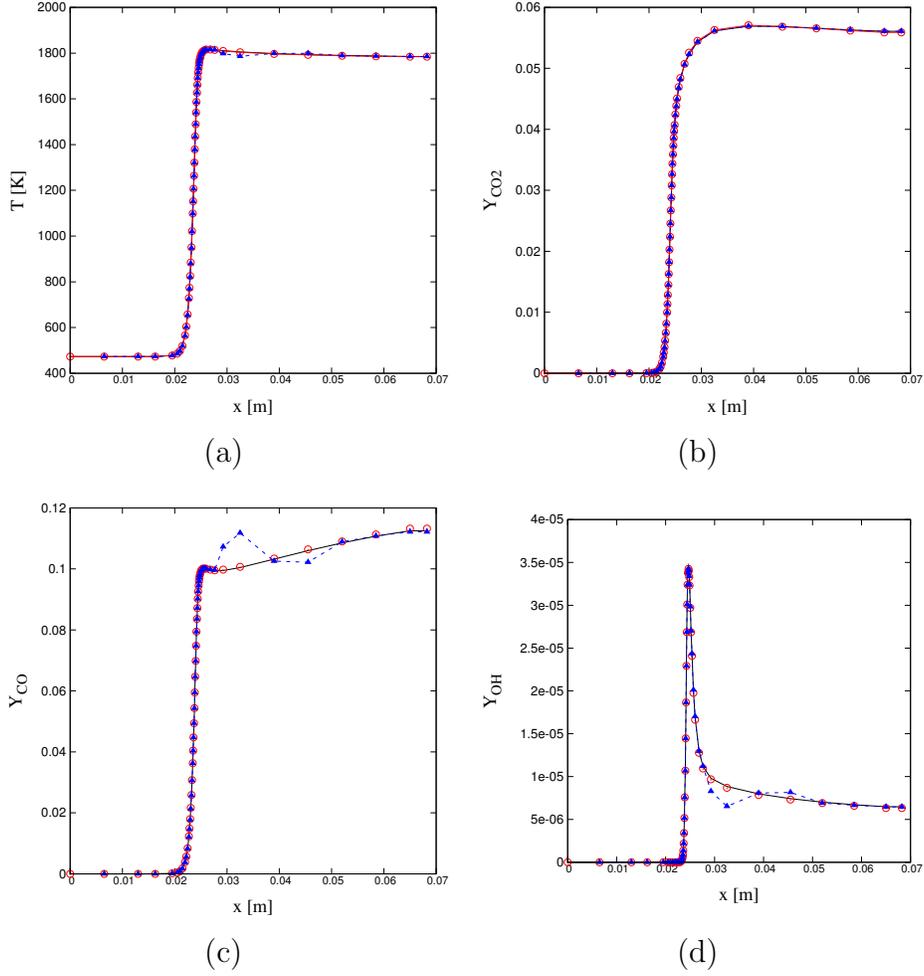


Figure 3: The structure of a freely propagating flame in CH_4 -air mixture at $\phi = 1.9$, $T_0 = 473$ [K], and $P = 1$ [atm] in the physical space; solid line: physical space solution; circles: solution retrieved from the previously generated flamelet table using the new definition of progress variable; triangles: solution retrieved from the previously generated flamelet table using $c = Y_{CO_2} + Y_{CO} + Y_{H_2O} + Y_{H_2}$. (a): temperature; (b): CO_2 mass fraction; (c): CO mass fraction; (d): OH mass fraction.

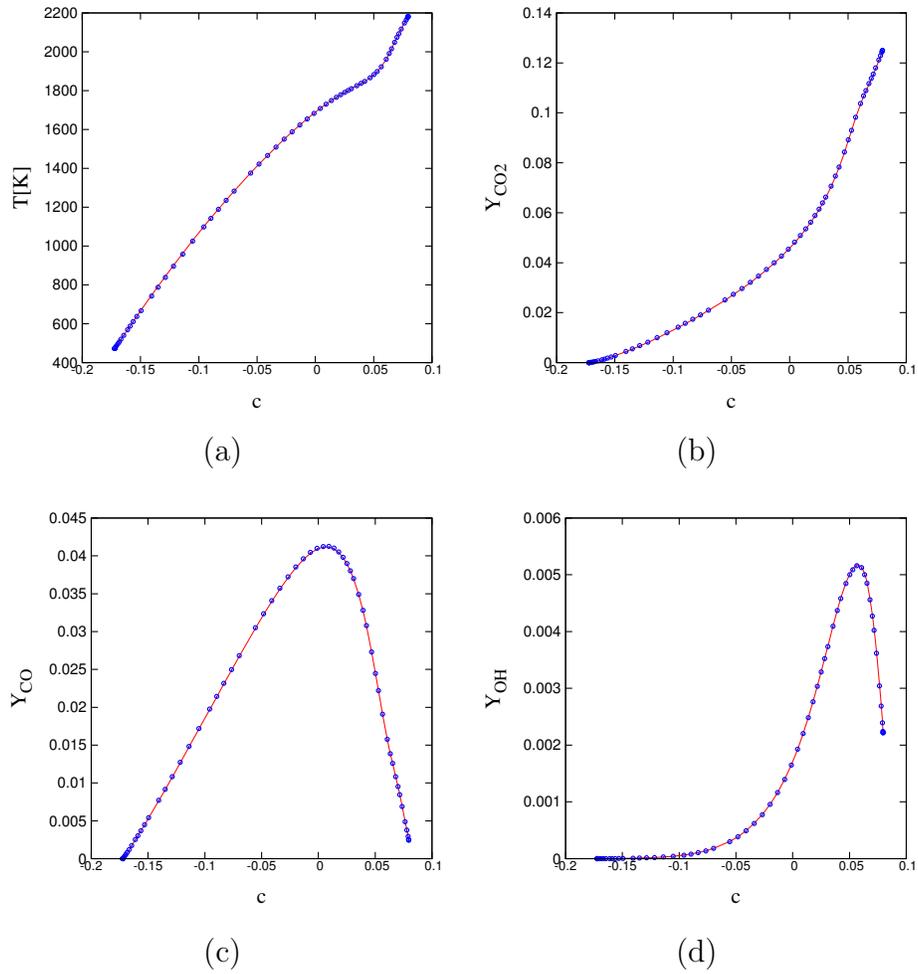


Figure 4: The solution of the flame, shown in Fig. 2 versus the progress variable; solid line: physical space solution; symbols: flamelet table. (a): temperature; (b): CO_2 mass fraction; (c): CO mass fraction; (d): OH mass fraction.

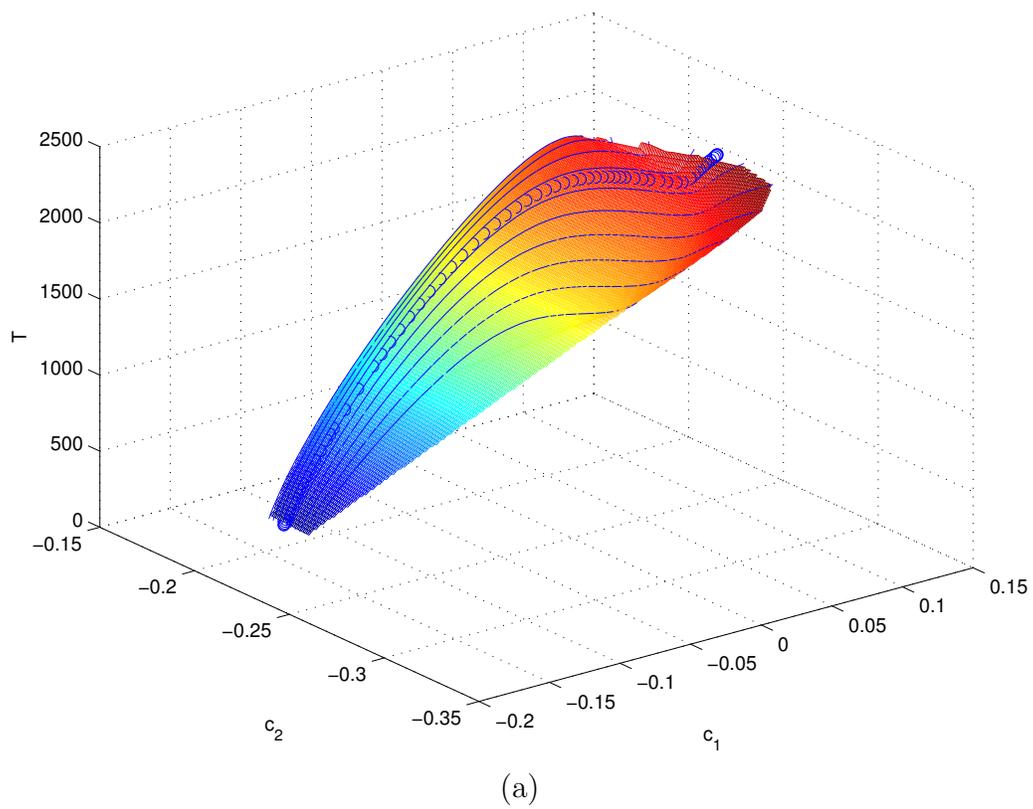


Figure 5: The temperature distribution in the progress variable space; solid lines: physical space solution for various equivalence ratios ; symbols: interpolated values for equivalence ratio $\phi = 1.15$.

H2	H	O	O2	OH
0.0066	0.0006	0.0030	-0.7767	0.0108
H2O	HO2	H2O2	C	CH
0.4345	-0.0002	-0.0000	0.0000	0.0000
CH2	CH(S)	CH3	CH4	CO
0.0000	0.0000	0.0008	-0.2191	0.1945
CO2	HCO	CH2O	CH2OH	CH3O
0.3491	0.0000	-0.0009	0.0000	0.0000
CH3OH	C2H	C2H2	C2H3	C2H4
-0.0002	0.0000	0.0011	0.0000	-0.0001
C2H5	C2H6	HCCO	CH2CO	HCCOH
0.0000	-0.0010	0.0000	0.0001	0.0000
N	NH	NH2	NH3	NNH
0.0000	0.0000	0.0000	0.0000	0.0000
NO	NO2	N2O	HNO	CN
0.0003	0.0000	0.0000	0.0000	0.0000
HCN	H2CN	HCNN	HCNO	HOCN
0.0000	0.0000	0.0000	0.0000	0.0000
HNCO	NCO	N2	AR	C3H7
0.0000	0.0000	-0.0031	-0.0000	0.0000
C3H8	CH2CHO	CH3CHO		
0.0000	0.0000	0.0000		

Table 3: The weight coefficients of each species, as obtained from PCA, to define the first progress variable, c_1 , for a premixed CH_4 -air flame at $\phi \in [0.6, 1.5]$. The results are shown up to the fourth decimal.

H2	H	O	O2	OH
0.0486	0.0002	-0.0083	-0.0785	-0.0252
H2O	HO2	H2O2	C	CH
0.1581	0.0006	0.0000	0.0000	0.0000
CH2	CH(S)	CH3	CH4	CO
0.0001	0.0000	0.0093	0.1589	0.6553
CO2	HCO	CH2O	CH2OH	CH3O
-0.6395	0.0001	0.0066	0.0000	0.0000
CH3OH	C2H	C2H2	C2H3	C2H4
0.0009	0.0000	0.0105	0.0001	0.0096
C2H5	C2H6	HCCO	CH2CO	HCCOH
0.0000	0.0077	0.0002	0.0028	0.0000
N	NH	NH2	NH3	NNH
-0.0001	0.0000	0.0000	0.0000	0.0000
NO	NO2	N2O	HNO	CN
0.0003	0.0000	0.0000	0.0000	0.0000
HCN	H2CN	HCNN	HCNO	HOCN
0.0000	0.0000	0.0000	0.0000	0.0000
HNCO	NCO	N2	AR	C3H7
0.0003	0.0000	-0.3190	0.0000	0.0000
C3H8	CH2CHO	CH3CHO		
0.0002	0.0000	0.0003		

Table 4: The weight coefficients of each species, as obtained from PCA, to define the second progress variable, c_2 , for a premixed CH_4 -air flame at $\phi \in [0.6, 1.5]$. The results are shown up to the fourth decimal.

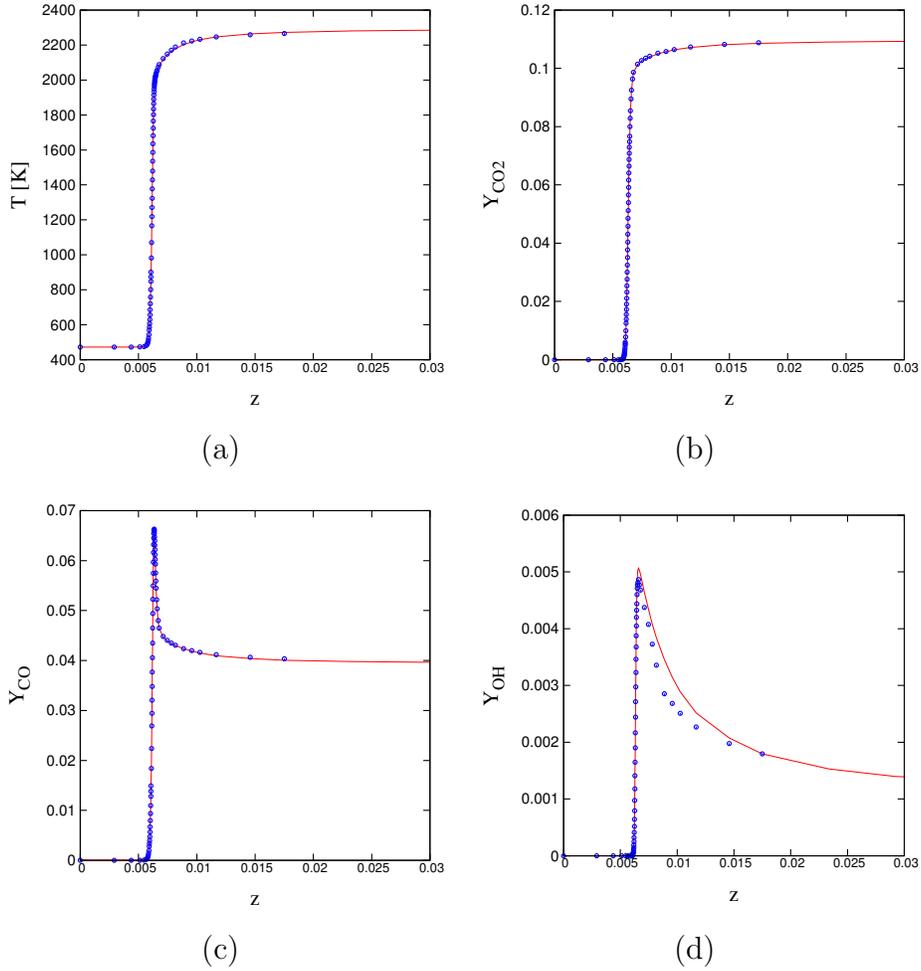


Figure 6: The structure of a freely propagating flame in CH_4 -air mixture at $\phi = 1.15$, $T_0 = 473$ [K], and $P = 1$ [atm] in the physical space; solid line: physical space solution; symbols: solution retrieved from the previously generated flamelet table. (a): temperature; (b): CO_2 mass fraction; (c): CO mass fraction; (d): OH mass fraction.