Turbulent reactive flow simulation with presumed β-PDF combustion model

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Introduction

The detailed understanding of different modes in turbulent deflagration is of fundamental and practical interest. The development of numerical methods with predictable capabilities is of primary interest for the study of turbulent reacting flow systems. In practical engineering and scientific calculations (industrial safety, combustion engines, etc.) a popular approach is to use simplified models for turbulence and chemical interactions. The simplest combustion models (as Eddy-Break-Up model) has demonstrated their ability to be a satisfactory choice for a number of practical simulations [1, 2], however the wide spectrum of combustion processes in application problems requires models with more solid theoretical background and applicability in a broader range of conditions.

A good compromise between model simplicity and its physical correctness is the 'presumed' probability density function (PDF) model. The presented work has the goal to introduce a new numerical technique for the efficient evaluations of mean reaction rates and to study numerically combustion of lean hydrogen-air mixtures using 'presumed' the β-PDF model.

Mathematical formulation

The mean reaction rate can be determined if the joint PDF F(T, **f**) (depending on temperature T and mass fractions f_1, f_2, … f_N,) is known

$$\overline{\dot{w}} = \iint\!\dots\!\int \dot{w}(T, f_1, f_2, \dots f_N) \cdot F(f_1, f_2, \dots f_N) dT df_1 df_2 \dots df_N .$$

If it is supposed that the temperature can be related to the composition of the mixture and that the chemical reaction can be described using one progress variable f, then the mean reaction rate reads as

$$\overline{\dot{w}} = \int \dot{w}(f) F(f) df .$$

The choice of the PDF has to be realistic in the combustion regimes of interest. In this work the 'presumed' β-PDF model for two-component mixing (N = 2) has been used. As a function on the (closed) interval [0,1] the expression for the β-PDF is given by [3]

$$F_{\beta_1,\beta_2}(f) = \begin{cases} \dfrac{\Gamma(\beta_1+\beta_2)}{\Gamma(\beta_1)\Gamma(\beta_2)} f^{\beta_1-1}\left(1-f^{\beta_2-1}\right), & 0 < f < 1; \\ 0, & f = 0,1; \end{cases}$$

with two strictly positive parameters β_1, β_2 and the standard Γ function. The evolution in time of these parameters is solely ruled by transport equations according to [4, 5].

The β-PDF is very popular since it can assume a wide variety of shapes, even approximate δ-functions, while being governed by two parameters only. Hence this model has the ability to adopt appropriate shapes for both fast mixing and fast chemical reaction, thus potentially covering both flamelet regime and thickened (thick) flames.

The chemical reaction rate is supposed to be describable by a one-step Arrhenius' Law

$$\dot{w} = k f^{\delta_0} (1 - f)^{\delta_1} \exp(-E / T(f)).$$

The evaluation of such integrals present serious numerical intricacies due to the singular behavior of the β-PDF at the points f = 0 or f =1 when β_1, $\beta_2 < 1$. Also very large parameters pose severe problems for standard numerical integration schemes.

To circumvent these difficulties, which cause standard numerical integration schemes to produce questionable results, a semi-analytical method for the approximate evaluation of such integrals has been proposed [6,7]. This method tries to avoid the evaluation of the β-PDF at nodes as much as possible

$$\overline{\dot{w}} = \int_0^1 \dot{w}(f) F(f, \beta_1, \beta_2) df \approx \sum_{j=1}^{p} C_j(\dot{w}) \Psi(\beta_1, \beta_2).$$

The coefficient-functions C_j, j = 1, … p (p = 22–26) have to be pre-calculated using about 120 – 170 predefined weights stored in matrices. The functions Ψ are fixed to a great extend and can be modified to avoid deteriorating accuracy at the ends of the domain of integration. The computational cost to obtain the functions C_j and Ψ appeared to be negligibly low compared to the costs of standard numerical integration schemes.

Special efforts were made to ensure the accuracy of the method especially at the singular points, since the β-PDF degenerates for very small parameter values to a linear combination of Dirac δ-functions, modeling infinitely fast combustion.

The mean reaction rate $\overline{\dot{w}}$ connected with an Arrhenius' Law can be displayed in a (m, s)-coordinate system, where the coordinates are defined by

$$s = \frac{1}{1 + \beta_1 + \beta_2}, \quad m = \frac{\beta_1}{\beta_1 + \beta_2}.$$

To demonstrate the characteristic features of the averaging process the following test function

$$g(x) = 180 \cdot (1 - x)^2 \cdot \exp\left(- \frac{1}{0.36x + 0.16(1 - x)} \right)$$

has been chosen.

The theoretical maximal absolute error of the method is equal to 10^{-3} – 10^{-8} depending on the properties of function $\dot{w}$. The computational costs of the procedure is about 140 – 190 multiplications and 11 – 13 function $\dot{w}$ evaluations according to the requirements on accuracy. The method allows varying the parameters of chemical kinetics including activation

energy, reaction rate constant and order of reaction, remaining with the same functions Ψ and the same set of weights. Due to its efficiency and flexibility the method allows a Fubini-type approach to evaluate double integral arising from, for instance, temperature dependent PDFs. The proposed method can be regarded as a highly efficient and very accurate alternative to table look-up or conventional numerical evaluation of integrals involving β-PDFs.

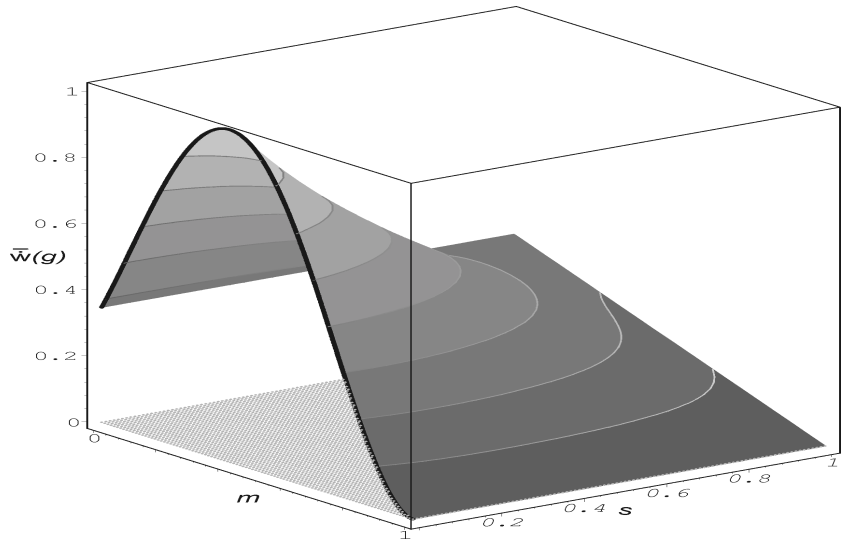

Fig. 1. The mean reaction rate $\overline{\dot{w}(g)}$ for the test function g versus the new variables m and s. $\overline{\dot{w}(g)}$ exhibits the correct 'boundary behavior' [7]; the thick line at the front end is the graph of the test function g.

Approximations of the global reaction rate available in the literature vary considerably with activation energy ranging from 8000 K to 18000 K (in different references) and are based either on experimental data (e.g. ignition delays) or on approximations of detailed kinetic schemes. Such ambiguity brings considerable uncertainty into the value of mean reaction rate, and, therefore, the reaction rate constants should be defined on the basis of additional considerations. In the present work an approach based on a regression procedure of experimental data on laminar flame speeds was proposed. It gave for lean-to-stoichiometric hydrogen-air mixtures (10 – 30% vol.) the following expression

$$\dot{w} = 1.8 \cdot 10^6 \frac{\rho}{\rho_0} f^2 \exp\left(\frac{-7553}{T}\right).$$

Experimental data

Experiments in an obstructed combustion tube were used to test the turbulent combustion model. The experiments were carried out in a cylindrical combustion tube of 12-m length and inner diameter equal to 35 cm, closed at both ends. The combustion tube was equipped with pressure transducers spaced 1 m apart along the total length of the tube. The instrumentation included also time-of-arrival diagnostics using infrared photodiodes spaced also 1 m apart. Annular obstacles with circular openings were located inside the tube. In all tests the distance between the obstacles was kept constant at 50 cm. The experiments chosen for simulation were performed with BR (blockage ratio) equal to 0.30 and the H_2 concentration of 15% and

10% vol. These two experiments exhibit different modes of flame propagation involving different physical phenomena. They constitute a good benchmark for the numerical model under consideration. In the first test case the fast acceleration of the flame up to DDT was observed, while in the second test case only slow combustion with a flame speed below 100 m/s occurred.

Numerical results and discussion

In the simulations of the experiments the geometry of the combustion tube was approximated using a cubic numerical grid with cell size equal to 1 cm. Such space resolution appeared to be sufficient to provide satisfying predictions for 15% H_2/air mixture if the EBU model is used. The same resolution was chosen to enable adequate comparison of the EBU and PDF models. The comparison of the simulation results with experimental data of two tests with 15% and 10% H_2 in air demonstrated the ability of the PDF model to predict all features of a combustion process (evolution of flame speed, velocities and amplitude of the generated pressure waves, etc.) reliably.

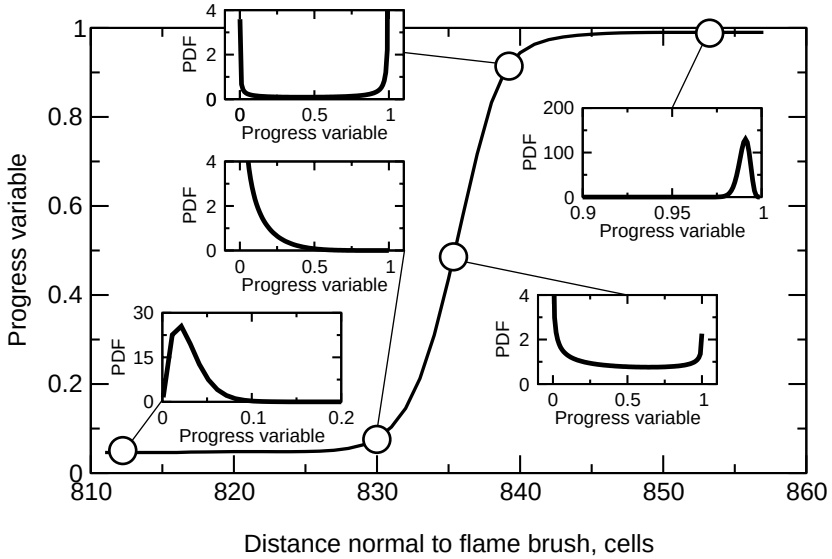

Fig. 2. Evolution of β-PDF in the flame brush depending on the progress variable value.

Note that if these experiments were simulated using the EBU model, in case of 15% H_2 usually good predictions were obtained, while for 10 % mixtures the EBU model fails.

The study of PDF evolution through the flame front in the case of a 15% mixture showed remarkable results concerning its behavior in the mixture. The appearing β-PDFs can be tallied into three clearly distinguished classes (Fig. 2) according to their shapes:

- before the flame front in a fresh mixture the PDF has Gaussian-type form (as it is defined by initial conditions, corresponding to the well-mixed case);
- in the flame brush it changes continuously to a U-shaped PDF, corresponding to the case when chemistry is faster than mixing;
- behind the reaction zone it slowly returns to a Gaussian-type form due to the mixing of products and reactants.

For the 10% mixture the PDF did not change its form, remaining Gaussian-like throughout the process, but noticeably broadening in flame brush.

These observations directly demonstrate the transient behavior of the β-PDF in case of accelerating flames in different combustion modes. The evaluation of Da (Damköhler number) for the slow case (10% H_2/air) gives values of about 0.5 in flame zone, hence confirming the assumption that thickened flames indeed occur in this case. In the fast case (15% H_2 in air) Da does not exceed 10^{-2} in the flame zone, which agrees well with observed U-shaped form of PDF (flamelet regime).

The comparison of the validity domain of the extended EBU model ($Re_t = 10^2$-10^6, Da = 0.08-$8 \cdot 10^{-4}$) [1] with the results of the present work brings to light that the validity domain of 'presumed' β-PDF model has a wider range of applicability near Da = 1 with respect to the EBU model, and that the model remains valid at least up to Da = 0.5.

Summary

Summarizing the results, it should be noticed that the proposed semi-analytical method of β-PDF integral evaluation makes it possible to perform detailed and high-accuracy simulations of reacting turbulent flows in complex geometries. Using this technique two combustion test cases in different combustion modes were simulated, directly demonstrating the transient behavior of β-PDF during the flame acceleration. Flamelet and thickened flame regimes have been clearly identified. The proposed approach has demonstrated good abilities to describe a wide class of combustion processes of practical interest.

References

1. A.S. Kotchourko, S. W. Breitung, and S. B. Dorofeev. Test of extended eddy break up model in simulations of turbulent H_2-air combustion. In: Proc. of the 17th ICDERS (Heidelberg, Germany, July 25-30, 1999), 1999, ISBN 3-932217-01-2, p p. 40.1-40.4
2. A. Kotchourko, W. Breitung, A. Veser, and S.B. Dorofeev. Tube experiments and numerical simulation on turbulent hydrogen-air combustion. In: Twenty First Symp. (Int.) on Shock Waves, pp. 3220.1-3220/6, Great Keppel Island, Australia, 1997.
3. R.K. Viertl. Einfuehrung in die Stochastik: mit Elementen der Bayes-Statistik und Ansaetzen fuer die Analyse unscharfer Daten. 2nd Edition. Springer, Vienna, 1997.
4. R. Borghi. Turbulent combustion modeling. Prog. Energy Combustion Sci., v. 14, pp. 245-292, 1988.
5. S.B. Pope. Statistical theory of turbulent flames. Trans. Royal Soc. London, v. 291, pp. 529-568, 1979.
6. B. Burgeth. The presumed β-PDF approach in turbulent combustion: An efficient calculation of mean reaction rates. In: Gemeinsames Arbeitsseminar des IKET (FZ Karlsruhe) und LKT (ETH Zürich), Editor: Müller, U., Yadigaroglu, G., Schulenberg, T., Techn. Report 32.21.05/A, Forschungszentrum Karlsruhe, pp. 37-43, 2000.
7. B. Burgeth. The Assumed PDF-Approach: Efficient Calculations of Integrals Involving the β-PDF. In: Abstracts of Work-in-Progress Posters, 28th Symposium on Combustion, The Combustion Institute. Edinburgh, Scotland, Jul. 30 – Aug. 4, 2000.