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State-of-the-art in premixed combustion modeling using flamelet generated manifolds

J.A. van Oijen *, A. Donini, R.J.M. Bastiaans, J.H.M. ten Thije Boonkkamp, L.P.H. de Goey

Eindhoven University of Technology, Eindhoven, The Netherlands

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ABSTRACT

Flamelet based chemical reduction techniques are very promising methods for efficient and accurate modeling of premixed flames. Over the years the Flamelet Generated Manifold (FGM) technique has been developed by the Combustion Technology Group of Eindhoven University of Technology. Current state-of-the-art of FGM for the modeling of premixed and partially-premixed flames is reviewed. The fundamental basis of FGM consists of a generalized description of the flame front in a (possibly moving) flame-adapted coordinate system. The basic nature of the generalized flamelet model is that effects of strong stretch in turbulent flames are taken into account by resolving the detailed structure of flame stretch and curvature inside the flame front. The generalized flamelet model, which forms the basis on which FGM is built, is derived in Part I. To be able to validate numerical results of flames obtained with full chemistry and obtained from FGM, it is important that the generalized flamelet model is analyzed further. This is done by investigating the impact of strong stretch, curvature and preferential diffusion effects on the flame dynamics as described by the local mass burning rate. This so-called strong stretch theory is derived and analyzed in Part I, as well as multiple simplifications of it, to compare the strong stretch theory with existing stretch theories. The results compare well with numerical results for flames with thin reaction layers, but described by multiple-species transport and chemistry. This opens the way to use the generalized flamelet model as a firm basis for applying FGM in strongly stretched laminar and turbulent flames in Part II. The complete FGM model is derived first and the use of FGM in practice is reviewed. The FGM model is then validated by studying effects of flame stretch, heat loss, and changes in elements, as well as NO formation. The application to direct numerical simulations of turbulent flames is subsequently studied and validated using the strong stretch theory. It is shown that the generalized flamelet model still holds even in case of strong stretch and curvature effects, at least as long as the reaction layer is dominated by reaction and diffusion phenomena and not perturbed too much by stretch related perturbations. The FGM model then still performs very well with a low number of control variables. Turbulent flames with strong preferential diffusion effects can also be modeled efficiently with an FGM model using a single additional control variable for the changes in element mass fractions and enthalpy. Finally FGM is applied to the modeling of turbulent flames using LES and RANS flow solvers. For these cases, the flame front structure is not resolved anymore and unresolved terms need to be modeled. A common approach to include unresolved turbulent fluctuations is the presumed probability density function (PDF) approach. The validity of this FGM-PDF approach is discussed for a few test cases with increasing level of complexity.

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* Corresponding author. Eindhoven University of Technology, Eindhoven, The Netherlands.
E-mail address: j.a.v.oijen@tue.nl (J.A. van Oijen).

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1. Introduction

Detailed numerical modeling of reacting flows has gained a continuous growth of interest in the last few decades. This is related to the fact that the development of new and the improvement of existing combustion equipment is getting more and more important. It has become strikingly clear that we cannot continue with the emission of undesired polluting combustion-byproducts in the way we have been doing in the last century, as this might lead to the destruction of our complete ecosystem. Engines, gas turbines and industrial furnaces play a major role in this emission and it is therefore of the utmost importance to improve the combustion properties of these systems significantly in the near future to avoid a further pollution of the atmosphere.

However, the improvement of combustion processes is a very difficult task: the improvement of one aspect often leads to a deterioration of other combustion aspects due to the complicated nature of combustion systems. For example, the shift of combustion technology during the last few decades toward much leaner low-NO_x premixed combustion processes in many applications has generally evolved in a reduction of the flame stability (leading e.g., to flame oscillations, noise, CO-emissions and even flame quenching). To be able to avoid all these problems, adaptations of combustion systems were needed, and to assist these studies, combustion CFD has become a very important tool. Another example is related to the demand for more sustainable combustion which has introduced a broad range of new fuels, some of which show really different combustion phenomena, for example hydrogen enrichment of fossil fuels from bio-sources introduces preferential diffusion phenomena which may have a huge impact on the structure and dynamics of underlying combustion processes. It is clear that combustion CFD is also very important to guide these developments. Therefore, further improvements by ad-hoc measures are insufficient and we have to rely on an in-depth understanding of the processes to be able to improve these systems significantly. Detailed experiments have to be carried out and detailed numerical modeling is needed to meet this goal. However, the numerical modeling of combustion systems is also very challenging from a scientific point of view. The interaction of the fluid flow, turbulence, chemical reactions and thermodynamics in reacting flows is of exceptional complexity. At the moment it has become within reach to model the most important physical aspects in detail, but this is still limited to small academic combustion problems. The modeling of the full details of practical combustion equipment will remain prohibitive in the next few decades, because of current and future limitations in computing power.

This problem asks for special treatments with respect to the modeling of flames. An important way to tackle this problem is by making use of the fact that the chemical time and length scales in most flames are very small. This idea can be exploited in different smart ways to reduce the number of equations to be solved, leading to an enormous reduction in computing effort. In the last decades two main routes have been followed using this idea in combustion science to model the detailed dynamics and structure of chemically reacting flows: chemical reduction techniques and laminar flamelet models.

Chemical reduction techniques – such as conventional reduction [1], Intrinsic Low-Dimensional Manifolds (ILDM) [2] and Computational Singular Perturbation (CSP) [3] – are based on the idea that most of the chemical time scales in the system are very small. If all transport processes are neglected, a time-scale analysis can be performed and the fastest time scales are assumed to be in steady-state. Mathematically, this means that all variables can be stored in a database as a function of a few controlling variables and during run-time only the equations for the controlling variables are solved. Large savings in computing time are reported by most methods with a small loss in accuracy.

Laminar flamelet methods [4] are based on the idea that flame structures are much thinner than most scales of the distortions in the flow, also implying that the chemical reactions are very fast compared to all other time scales. For that reason, the internal structure of the flame front is almost frozen while it moves around in the flow