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Differential diffusion effects inclusion with flamelet generated manifold for the modeling of stratified premixed cooled flames

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Abstract

CFD predictions of flame position, stability and emissions are essential in order to obtain optimized combustor designs in a cost efficient way. However, the numerical modeling of practical combustion systems is a very challenging task. As a matter of fact, the use of detailed reaction mechanisms is necessary for reliable predictions, especially for highly diffusive fuels. Unfortunately, the modeling of the full detail of practical combustion equipment is currently prohibited by the limitations in computing power, given the large number of species and reactions involved. The Flamelet Generated Manifold (FGM) method reduces these computational costs by several orders of magnitude without loosing too much accuracy. Hereby, FGM enables the application of reliable chemistry mechanisms in CFD simulations of combustion processes. In the FGM technique the progress of the flame is generally described by a few control variables. For each control variable a transport equation is solved during run-time. The flamelet system is computed in a pre-processing stage, and a manifold with all the information about combustion is stored in a tabulated form. In the present paper, the FGM model is implemented for the analysis of partially premixed non-adiabatic flames, including the effects of differential diffusion. Subsequently, a computational analysis of partially premixed non-adiabatic flames is presented. In this scope, a series of test simulations is performed using FGM for a two dimensional geometry, characterized by a distinctive stratified methane/air inlet, and compared with detailed chemistry simulations. The results indicate that detailed simulations are well reproduced with the FGM technique.

Keywords: Differential diffusion; Flamelet generated manifolds; Heat loss; Mixture fraction; Premixed

1. Introduction

In industry the development of clean and efficient technologies for the combustion process is achieved by a combination of experimental and numerical research. Experimental testing is in general extremely expensive, and a great reduction of the costs could be made by maximizing the usage of simulations in the design phase. Unfortunately, the modeling of the full detail of practical combustion equipment is currently prohibited by the limitations in computing power, given the large

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number of species and reactions involved. The Flamelet-Generated Manifold (FGM) [1] method, also referred to as Flamelet Prolongation of ILDM [2], reduces these computational costs by several orders of magnitude without loosing too much accuracy. Hereby FGM enables the application of reliable chemistry mechanisms in CFD simulations of combustion processes. The approach is based on the idea that the most important aspects of the internal structure of the flame fronts should be taken into account. In the FGM technique the course of the reaction is defined in terms of a few control variables, for which transport equations are solved during runtime. And here lies one of the main strengths of the FGM technique, which is that the number of independent control variables can be increased for a better description of the combustion phenomena. This means that, starting with a single reaction progress variable, the accuracy of the method can be straightforwardly extended for the inclusion of heat loss, mixture fraction and differential diffusive effects, as shown in the following section. The flamelet system is computed in a pre-processing stage, and a manifold with all the information about combustion is stored in a tabulated form. To this purpose a laminar flamelet database is generated from a one-dimensional flamelet calculation performed with full kinetics and detailed transport. The FGM technique has proven to be very accurate for laminar premixed Bunsen flames including heat loss effects [1], highly stretched premixed counter-flow flames [3] and confined triple flames [4]. This technique performed well also in DNS of a turbulent expanding flame [5], showing that a single control variable can give accurate predictions on the local mass burning rate. Recently the approach has proven to be appropriate also for the computation of turbulent partially premixed flames [6,7], also with heat loss [8]. A large part of current combustion models adopt a unity Lewis number assumption, imposing that mass and heat diffuse at an equal rate in the flame. On the opposite, when *Le* is not equal to one, species and heat locally redistribute. This phenomenon is also referred to as differential diffusion [9]. The inclusion of this effect is important especially in the case of laminar flames. With the purpose of including every aspect in the numerical modeling of differentially diffusive flames, in this paper the FGM model is extended for differential diffusion inclusion and applied to cooled stratified premixed flames by means of a 3D manifold where the control variables are represented by the progress variable $\mathcal{Y}$, enthalpy h and mixture fraction Z. The combined inclusion of these effects represents a challenge. At the best of the authors' knowledge, the application of FGM in combination with heat loss, mixture fraction variations and differential diffusion effects has never been studied in literature. Such implementation of the FGM technique is therefore applied for two-dimensional test case flame simulations with stratified inlet and accurately compared with detailed chemistry computations. The results of the present validation are supported and further motivated by the detailed Le = 1 comparison given in [10] for the same geometry and conditions. The fuel adopted for the simulations is methane, because of its mild diffusivity. In fact, the work presented in this paper represents a test and validation of the method, as a first and necessary step before considering highly diffusive fuels such as hydrogen.

2. The FGM database generation

In the FGM technique the whole chemistry is directly retrieved from a laminar flamelet database generated from multiple one-dimensional flamelet calculations performed with detailed kinetics and transport. In this study cooled stratified premixed methane/air combustion is considered, at atmospheric pressure conditions. The FGM consists of a 3D manifold in which the control variables are represented by the progress variable $\mathcal{Y}$, enthalpy h and mixture fraction Z. The minimal dimension of the manifold in the phase space is determined by an accuracy assessment [11], however several automated techniques have been recently proposed, e.g. [12,13]. As described in the introduction, differential diffusion results in local changes in mass fraction and enthalpy. In order to accurately predict such effect, mass fraction and enthalpy must be included as control variable of the FGM description. The progress variable $\mathcal{Y}$ is defined as a linear combination of species mass fraction: $\mathcal{Y} = \sum_{i=1}^{N_s} \alpha_i Y_i$,where Y_i is the mass fraction of specie i and N_s the total number of species. The weighting coefficients α_i are arbitrarily chosen, with the only restriction of ensuring a monotonic profile of $\mathcal{Y}$ in the whole interval between the unburned mixture and the chemical equilibrium. For the calculations described in this paper, it is chosen: $\alpha_{CO_2} = M_{CO_2}^{-1}, \alpha_{H_2} = M_{H_2}^{-1}, \alpha_{H_2O} = M_{H_2O}^{-1}, \alpha_{O_2} = M_{O_2}^{-1}, \alpha_i = 0 \; \forall \; i \notin \{CO_2, H_2, H_2O, O_2\}$, in which M_i is the molar mass of element i. Heat loss to the combustion chamber walls cause enthalpy not to be conserved throughout the domain. In order to take this into account in the tabulation process, the laminar flamelets have to be solved for different values of enthalpy, introducing enthalpy h as a control variable. The flamelets are computed as steady, fully premixed, flat flames, for a given pressure, composition and temperature of the inlet mixture. At the burned side (chemical equilibrium) Neumann type boundary conditions are imposed instead. The procedure for the creation of enthalpy-decreasing set of flamelets might be