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LES combustion modeling using the Eulerian stochastic field method coupled with tabulated chemistry

Amer Avdić[a], Guido Kuenne[a], Francesca di Mare[b], Johannes Janicka[a,*]

[a] Institute of Energy and Power Plant Technology, TU Darmstadt, Jovanka-Bontschits-Strasse 2, Darmstadt 64287, Germany
[b] Institute Reactive Flows and Diagnostics, TU Darmstadt, Jovanka-Bontschits-Strasse 2, Darmstadt 64287, Germany

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ABSTRACT

In this work a transported joint scalar probability density function method is combined with the flamelet generated manifolds (FGM) tabulated chemistry approach for large eddy simulation (LES) modeling of turbulent combustion. This strategy accounts for the turbulence-chemistry interaction at reasonable computational costs and allows the usage of detailed chemistry information by tabulation. Apart from the details regarding the solution procedure, a technique for an improved stability of the proposed approach is introduced and validated using a one-dimensional test case. Next, a two-dimensional flame configuration is considered in order to perform an in-depth analysis regarding the laminar and turbulent behavior of the model. Here, transient and time-averaged simulation data is used to provide insight into the predicted flame shape and its dynamics, where the implemented approach is compared with the well-established artificially thickened flame (ATF) combustion model. Moreover, the sensitivity of the results to different modeling approaches and model parameters is investigated. Finally, the method is applied to a three-dimensional turbulent stratified burner. Here, in addition to the ATF model, the suggested approach is compared to measurements of the velocity and scalar quantities to evaluate its prediction capability. Consequently, the investigation conducted in this work aims to provide a complete picture on the ability of the proposed method to reproduce the flame propagation and the resulting flow conditions within complex premixed and stratified turbulent flames.

1. Introduction

The permanent increase of computer resources has ensured that the large eddy simulation (LES) rationale becomes a commonly used computational tool for the prediction of complex turbulent reacting flows. This approach represents the best compromise between practicality and physical accuracy, since the turbulent motion associated with the large, energy-containing eddies is computed directly, whereas the effects of the smallest ones are modeled. Accordingly, the LES methodology enables capturing the unsteady processes connected to turbulent combustion, but at the same time the typical LES grid size is too large in order to fully resolve all of the turbulent and scalar structures. Accordingly, an important part of the flame-turbulence interaction evolves on the sub-grid scale making its characterization difficult. Additionally, a large number of elementary reactions involved in the combustion process need to be considered for a realistic description of the chemistry, which can yield extensive computational requirements for the numerical simulations of complex systems. Consequently, the application of detailed reaction mechanisms in the context of LES and complex configurations is currently not feasible.

Therefore, the objective of the combustion models is to reproduce the most important flame properties on the LES mesh. In the context of the premixed flames, these are the flame propagation speed and its wrinkling caused by the turbulence. There are well-known approaches for the description of the premixed flames such as G-equation [1], the flame surface density [2], filtered tabulated chemistry for LES (F-TACLES) [3], and the artificially thickened flame (ATF) model [4]; an overview of recent strategies is provided by Janicka and Sadiki [5] and Pitsch [6]. Furthermore, tabulated chemistry models have proven to be successful in strongly reducing the computational effort compared to detailed reaction mechanisms by using a small number of controlling variables. Here, the tabulated models also include the detailed information on species within the flame, in contrast to strongly reduced reaction mechanisms with a comparable number of transport equations solved. As the tabulation is conducted prior to the LES, assumptions need to be introduced regarding the flame structure. Namely, approaches

* Corresponding author.
E-mail address: janicka@ekt.tu-darmstadt.de (J. Janicka).

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Nomenclature

C_s	Smagorinsky coefficient
C_Ω	micro-mixing constant
C_w	weighting modification constant
dW_j^n	nth Wiener process in j direction
$\mathcal{E}$	efficiency function
$\mathcal{F}$	joint probability density function
$\mathfrak{F}$	thickening factor
$\mathcal{G}$	spatial filtering operator
h	specific enthalpy of the mixture
I	turbulence intensity
L_F	flame length
Le	Lewis number
m	mass
N	number of stochastic fields
N_α	number of table controlling variables
$\mathcal{O}$	in the order of
$\mathcal{P}$	probability density function
Pr	Prandtl number
s	coordinate in the flame reference frame
S_{ij}	rate of strain
Sc	Schmidt number
s_L	laminar flame speed
s_L^0	laminar flame speed without flame stretch
s_N	flame speed in normal flame direction
T	temperature
t	time
u_j	velocity in j direction
w	weighting factor
x, y, z	spatial coordinate
Y	mass fraction
$\mathcal{Z}$	mixture fraction
δ_{ij}	Kronecker-symbol
Δ	grid size
Δ_t	time step size
$\zeta(0, 1)$	dichotomic vector
μ	dynamic viscosity
ν	kinematic viscosity
ξ_α^n	nth stochastic field of the scalar α
ρ	density
τ_{ij}	components of the viscous stress tensor
τ_{sgs}	sub-grid mixing time scale
φ	arbitrary quantity
ϕ	general species/scalar
χ	scalar dissipation rate
ψ	sample or composition space of the species/scalar
Ω_{sgs}	sub-grid mixing time
$\dot{\omega}$	chemical source term
$\cdot^*$	auxiliary variable for stability
$\cdot_\alpha$	table controlling variable
$\cdot_{ac}$	accumulated
$\cdot_b$	burnt state
$\cdot_m$	species
$\cdot_{max}$	maximum
$\cdot_{sgs}$	sub-grid scale
$\cdot_u$	unburnt state

such as the steady flamelet concept or the flamelet generated manifolds (FGM) are bound to certain combustion modes, in particular non-premixed [7,8] or premixed flames [9,10], depending on the underlying flamelets.

In the context of the LES, the knowledge of the one-point joint sub-grid probability density function (sub-grid PDF - in the literature also termed as filtered density function FDF) for the scalar quantities can provide an alternative approach to represent the turbulence-chemistry interaction. A presumed shape of sub-grid PDF applied to situations of complex mixing or strong turbulence-chemistry interaction with multiple scalars is often a too restrictive approximation. Namely, when assuming a generic sub-grid PDF shape, the scalar fluctuations due to convection caused by all turbulent scales, molecular diffusion, and chemical reaction are inherently presumed and do not consider the physical processes taking place [11]. Moreover, an assumption that all scalar distributions are statistically independent is physically incorrect, which becomes significant with an increasing number of table controlling variables [12]. The more elaborate approach is to solve a modeled form of the equation governing the time evolution of the joint sub-grid PDF, whereby a description of the filtered and the sub-grid scalar fields can be obtained. One of the advantages related to the formulation of this method is that the chemical source term is in a closed form. On the other hand, the arising molecular mixing term needs to be modeled. Here, the dynamics of both, chemistry and molecular mixing influence the shape of the joint sub-grid PDF. Generally, due to the high dimensionality of the transported joint sub-grid PDF, a finite-volume discretization is impracticable. Instead, the equation can be represented by using less computationally demanding stochastic Monte Carlo (MC) solution methods in which the sub-grid PDF is represented by either stochastic particles or fields, i.e. obtained by a set of stochastic differential equations.

In the formulated methods by Valiño [13] and Sabel'nikov and Soulard [14] smooth stochastic fields are used to represent the sub-grid PDF undergoing diffusion, turbulent convection, and chemical reaction. The practical advantage of these methods is that the resulting stochastic fields are continuous and differentiable in space and continuous though not differentiable in time. As a consequence, there are no spatially varying sampling errors in the evaluation of statistical moments, which are easy to compute. Up to now, the LES studies employing the Eulerian stochastic field method were applied to laboratory jet flames [15], non-premixed [16] and partially premixed burners with auto-ignition [17–19] as well as to complex premixed burners [20,21]. In the previous studies, this method is used only in conjunction with reduced mechanisms.

The aim of the present work is to further extend the Eulerian stochastic field (ESF) method in the context of the FGM approach, which will serve as a chemistry reduction strategy. Herein, a three-dimensional chemistry table will be used. This novel approach is expected to significantly reduce the computational costs associated with the application of the method, whereby the production of the chemical database using detailed mechanisms can increase the prediction potential of the model. More specifically, as some major species with monotonic behavior generally serve as the FGM table controlling variable, the resolution requirements for prediction of minor species will therewith reduce. Still, by design, the table contains the states as produced by the full reaction scheme and therefore guarantees that vital properties are recovered in the FGM approach. Particularly those are the correct flame speed for the full range of parameters, accurate burnt gas conditions as well as a proper representation of most species involved. The specific objectives of this work are: (i) to develop an approach that combines the Eulerian stochastic field method with the FGM chemistry reduction strategy, (ii) to conduct a comprehensive study on the model performance, and finally (iii) to evaluate the capability of the joint ESF-FGM in simulating a complex premixed and stratified flame, for which detailed scalar and velocity measurements are available. This paper is organized as follows. In Section 2 the LES solver and the employed turbulence modeling are outlined. This is followed by the introduction of the combined ESF-FGM approach

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