Combustion and Flame 161 (2014) 525–540

Contents lists available at ScienceDirect

Combustion and Flame

journal homepage: www.elsevier.com/locate/combustflame

Assessing LES models based on tabulated chemistry for the simulation of Diesel spray combustion

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ARTICLE INFO

Article history:
Received 19 September 2012
Received in revised form 4 September 2013
Accepted 11 September 2013
Available online 14 October 2013

Keywords:
Large-eddy simulation (LES)
Chemistry tabulation
Turbulent combustion
Autoignition
Nonpremixed combustion
Flamelet modeling
Diesel combustion

ABSTRACT

In the context of large-eddy simulation (LES) of Diesel engine combustion, two LES combustion models are proposed. Their ability to predict autoignition delays and heat release of an autoigniting liquid α-methylnaphthalene/*n*-decane jet injected into a constant-volume chamber under Diesel-like conditions is assessed. These models retain the tabulation of a complex chemistry scheme using autoigniting homogeneous reactors (HR) at constant pressure. This allows accounting for the chemical complexity of heavy hydrocarbon fuels over the wide range of conditions representative for Diesel engines, at comparatively low CPU time overhead. The tabulated homogeneous reactor (THR) approach assumes the local structure of the reaction zone to be that of an HR, while the approximated diffusion flame (ADF) approach is based on autoigniting strained diffusion flames. Two variants of each approach are considered, either neglecting sub-grid-scale mixture fraction variance (THR and ADF models), or accounting for it via a presumed β-PDF (THR-pdf and ADF–PCM models). LES results indicate that the ADF model assuming diffusion flame structures tends to predict faster propagation of the combustion toward less reactive mixture fractions then the THR model. Moreover, neglecting the mixture fraction fluctuations strongly overestimates initial experimental heat release rates after autoignition. Comparison between models shows that this assumption yields higher reaction rates and temperature levels close to the stoichiometric mixture fraction zones. Predictions in terms of autoignition are remarkably close with all models, and exhibit very few variations from one realization to the other. Variations in global heat release rate become more apparent for different realizations at later instants, in relation to the interaction of large flow scales with combustion.

1. Introduction

The simulation of Diesel spray combustion by computational fluid dynamics (CFD) is a very challenging task. It requires modeling and simulating transient liquid fuel injection at very high pressures. The resulting spray formation and evolution lead to a highly turbulent stratified flow in which the fuel evaporates, mixes with the gases present in the cylinder, and finally auto-ignites and burns. Furthermore, the high-order hydrocarbon fuels most commonly used in Diesel engines exhibit a negative temperature coefficient (NTC) region resulting from competition between low- and high-temperature chemistry [1]. The use of detailed chemistry to predict these effects is therefore mandatory, and the kinetic schemes must be able to predict combustion chemistry over the wide ranges of mixture fraction, temperature, pressure, and dilution rate typical of Diesel engines.

A wealth of research has been dedicated to simulating Diesel-type sprays, resulting in a broad range of combustion models able to reproduce with acceptable accuracy autoignition delays, liftoff lengths, heat release, and pollutant emissions. Most of these models were formulated in the frame of a Reynolds-averaged Navier–Stokes (RANS) approach [2]. More recently, large-eddy simulation (LES) has received increasing interest [3,4], as it is believed to allow more accurate prediction of the unsteady and highly stratified flow conditions found in Diesel sprays. This is a direct consequence of the fact that LES simulates local, instantaneous, spatially filtered flows, resolving the largest flow scales and modeling only the effects of the smallest ones. In addition to improved predictivity, it potentially allows addressing noncyclic phenomena not accessible to RANS.

An approach widely used to account for complex fuel chemistry in Diesel combustion simulations, in either RANS or LES formalisms, is to directly solve for it within a CFD code. Jhavar et al. [5] applied such an approach to the LES of a HCCI engine, and Li et al. [3] to the LES of a conventional Diesel engine. A major drawback of this method is the large CPU time required to solve the

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http://dx.doi.org/10.1016/j.combustflame.2013.09.006

chemistry online and to transport all the required chemical species. Therefore such approaches use reduced chemical schemes with a domain of validity that is often much smaller than of detailed schemes, and rely on coarse CFD meshes to limit CPU time requirements. Furthermore, no closure is considered to describe the interactions between turbulence and chemistry. The conditional moment closure (CMC) approach [6] addressing this point by solving balance equations for moments conditioned on the mixture fraction has successfully been applied to RANS [7] and LES [4] computations of Diesel combustion. In terms of practical usage, however, CMC formalism requires high computational overhead, especially for detailed chemical schemes. Another approach to represent turbulence chemistry interactions consists in transporting a probability density function (PDF) as performed by Pei et al. [8] on a *n*-heptane jet under Diesel engine conditions. They compared a well-mixed model with a transported PDF model, showing that the latter provided better overall results, which seems to underline the importance of turbulence–chemistry interactions in Diesel jets.

An alternative approach is to retain the flamelet assumption [9,10] to model turbulent nonpremixed flames. The representative interactive flamelet (RIF) model [11,12] uses this assumption and computes one [12] or several [13] laminar diffusion flames using a dedicated flamelet code coupled online to the CFD code. This approach has widely been used for RANS computations of Diesel combustion [13,14], but remains very time-consuming when applied to detailed chemical schemes.

A solution to overcome this limitation is to use a flamelet/progress variable (FPV) approach [15]. Its principle is to generate a priori a flamelet lookup table with a reduced number of input parameters. During the computation the lookup table is used in the CFD code to estimate the species reaction rates. The advantage of this tabulation approach is that the resolution of the chemistry is done prior to the CFD computation, so that the computational overhead is very small: this approach only requires the transportation of a few chemical species in the CFD code, and the resolution of complex schemes is replaced by interpolations in a lookup table with few parameters. A β-pdf is assumed for the mixture fraction distribution. Pierce and Moin [15] performed LES computations of a coaxial jet combustor and obtained satisfactory results using steady state flamelets. In order to avoid explicit dependence on a flamelet time scale, Ihme et al. [16] proposed the unsteady flamelet/progress variable (UFPV) model based on unsteady flamelets. They reported a significant improvement of autoignition delays in their LES as compared to a steady flamelet approach. Using a similar approach based on tabulated unsteady flamelets with a progress variable based on the enthalpy, Lehtiniemi et al. [17] performed RANS calculations of a Diesel-type spray. Depending on the configuration, many flamelets may have to be resolved for different initial conditions to produce a complete lookup table. This generation can become excessively CPU-time-consuming and even outrun memory capacities if applied with detailed chemical schemes. For this reason, the ADF–PCM model [18,19] tabulates approximated diffusion flames. It consists in resolving the flamelet equation only for the progress variable and extracting reaction rates and species from a pretabulated homogeneous reactor lookup table. This allows both reducing the computational time required to build the lookup tables and using detailed chemical schemes.

The characteristic scales of turbulent mixing and chemistry may vary greatly within a cycle or from one engine type to another, depending on the injection strategy used. Lee et al. [20,21] applied a combination of models for addressing three main types of Diesel combustion: the Shell model [22] for autoignition, a characteristic time combustion model for the premixed phase [23], and a tabulated steady flamelet model for nonpremixed combustion. The transition between premixed and nonpremixed combustion is performed based on the local Damköhler number. Hu et al. [24] performed simulations of conventional and HCCI Diesel modes with the extended flamelet time scale (EFTS) model [25] coupled with a reduced chemistry scheme for the autoignition modeling. The ETFS approach consists in relaxing flamelet species toward equilibrium with a pretabulated relaxation time that is a function of mixture fraction. Hu et al. [26] also reported a similar approach based on the distinction between kinetically controlled, quasi-steady homogeneous, and quasi-steady flamelet combustion for conventional engines. A difficulty of such approaches is the definition of the transitions between different models based on criteria that lack generality, which can be expected to lead to a lack of predictive accuracy [27].

The application of LES to Diesel spray combustion is as yet very limited, and most of the published work relies on using RANS CFD codes and coarse grids, simply replacing RANS turbulence models with sub-grid-scale LES models [4,5,26]. Although predictions were found accurate, this ad-hoc approach does not allow fully exploiting the improved predictive capability of LES, as it relaxes its specific requirements in terms of numerical accuracy and spatial resolution.

The purpose of the present study is to assess the ability of two nonpremixed LES combustion models based on offline chemistry tabulation to predict Diesel spray combustion using the AVBP CFD code [28]. Liquid spray and sub-grid-scale models, as well as a numerical setup, are specifically tailored to fulfill LES requirements. The assessed combustion models offer the advantage of accounting for complex chemistry effects, while leading to small CPU time overheads when used in the LES code. Both these characteristics are of crucial importance for future practical applications to full Diesel engine LES.

Two different types of combustion models are proposed in the present paper. A first approach assumes that the sub-grid-scale structure of the reaction zone corresponds to a homogeneous reactor (HR), thus neglecting sub-grid-scale mixing effects. A second approach is to account for these effects by assuming the sub-grid-scale structure to be that of a strained diffusion flame. Both these approaches are proposed in two variants, depending on the form of the presumed mixture fraction PDF used to describe sub-grid-scale mixture fraction stratification effects. They are then implemented into the LES flow solver AVBP and applied to the simulation of a Diesel-type jet experiment.

Section 2 starts by setting the LES modeling framework, describing the set of transport equations used for the gaseous phase, briefly outlining the spray description based on a mesoscopic Eulerian formalism, and presenting the LES closures used for the unknown convection, evaporation, and mixing terms. Section 3 proposes a detailed description of the two proposed combustion models. After their common principles are outlined, details are given on their formulation, adaptation to the LES context, and integration into the CFD code. Section 4 presents a first application of the developed approach to the LES of a liquid spray composed of 30% α-methylnaphthalene and 70% *n*-decane injected into a constant-volume chamber under conditions representative of pilot Diesel injection. First, the experimental setup studied by Bruneaux [29] is described, before the numerical configuration is detailed using the AVBP LES code [28] and the imposed boundary conditions for the Eulerian liquid jet model. An analysis of the quality of the LES results is also presented and discussed. Finally, Section 5 discusses the LES results, assessing the predictive capability of the discussed combustion models and variants.

2. Basic equations

A perfect gas mixture composed of N species is considered. The turbulent flow is described by the compressible reactive