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Simulations of spray autoignition and flame establishment with two-dimensional CMC

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Abstract

The unsteady two-dimensional conditional moment closure (CMC) model with first-order closure of the chemistry and supplied with standard models for the conditional convection and turbulent diffusion terms has been interfaced with a commercial engine CFD code and analyzed with two numerical methods, an "exact" calculation with the method of lines and a faster fractional-step method. The aim was to examine the sensitivity of the predictions to the operator splitting errors and to identify the extent to which spatial transport terms are important for spray autoignition problems. Despite the underlying simplifications, solution of the full CMC equations allows a single model to be used for the autoignition, flame propagation ("premixed mode"), and diffusion flame mode of diesel combustion, which makes CMC a good candidate model for practical engine calculations. It was found that (i) the conditional averages have significant spatial gradients before ignition and during the premixed mode and (ii) that the inclusion of physical-space transport affects the calculation of the autoignition delay time, both of which suggest that volume-averaged CMC approaches may be inappropriate for diesel-like problems. A balance of terms in the CMC equation before and after autoignition shows the relative magnitude of spatial transport and allows conjectures on the structure of the premixed phase of diesel combustion. Very good agreement with available experimental data is found concerning ignition delays and the effect of background air turbulence on them.

Keywords: Conditional moment closure; Autoignition; Turbulent; Spray

1. Introduction

Simulation of autoignition for liquid fuel sprays under diesel engine conditions has attracted the attention of numerous researchers in the past decades. There is a recent resurgence of interest in this activity due to the emergence of homogeneous charge compression ignition (HCCI) engines, which rely on autoignition of mixtures of varying inhomogeneity. Apart from the modeling challenges related to the complex spray dynamics, appropriate treatment of the turbulence–chemistry interaction is needed for both conventional diesel and HCCI engines. The well-known closure problem of the species chemical source terms has led to a variety of modeling approaches. The simpler ones are based on so-called

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Nomenclature

Y_α	Mass fraction of species α
T	Temperature
h	Enthalpy
Q_α	Conditional mean of mass fraction Y_α of species α
Q_T	Conditional mean of temperature T
w_α	Conditional chemical reaction term of species α
w_h	Conditional chemical reaction term of enthalpy
u_j	Velocity components, $j = 1, \ldots, 3$
x_j	Cartesian coordinates, $j = 1, \ldots, 3$
c_P	Specific heat capacity at constant pressure
D	Diffusion coefficient
N	Scalar dissipation
P	Pressure
R	Universal gas constant
MW_η	Mean molar mass
Sc	Schmidt number
Le	Lewis number
ξ	Mixture fraction or conserved scalar
ρ	Density
η	Sample space variable for ξ
χ	Mean scalar dissipation rate
ω	Reaction rate of species
μ	Viscosity
k	Turbulent kinetic energy
ε	Eddy dissipation rate

Subscript indices

t	Relating to turbulence
α	Species index
η	Conditioned on $\xi = \eta$
MR	Most reactive
st	At stoichiometry

Superscript indices

$''$	Fluctuation with respect to conditional mean

Overbar symbols

$\sim$	Favre averaging
$-$	Conventional averaging

characteristic time scales [1] and require additional modeling to treat the ignition process [2,3]. Despite strong simplifications, these models can be effectively employed to obtain engineering quantities for a broad range of engine sizes [4] given careful consideration of model constants.

Recently, more advanced models have become increasingly popular as they offer a promising way to treat the turbulence–chemistry interaction and allow inclusion of complex chemistry. Flamelet models [5,6], originally based on precalculated lookup tables, have been successfully applied to study spray diffusion flames [7] and extended to engines [8]. The representative interactive flamelet (RIF) model, which uses two-way coupling between the flow-field solver and the transient flamelet integration, has seen highly successful use for autoignition of fuel sprays in combustion chambers [9] as well as in engines [10–12]. However, using one flamelet to represent the entire domain was found to be insufficient to accurately predict the premixed stage of the combustion and, in particular, heat-release rates, which poses problems in pollutant formation computation. Newer developments based on the Eulerian particle flamelet model (EPFM) [13,14] therefore employ multiple RIFs and additionally solve an Eulerian transport equation to obtain the probability of finding the corresponding flamelet in each cell. More complex situations such as those with pilot injection have also been treated successfully with a flamelet formulation with two mixture fractions [15]. Alternative developments employing presumed PDFs and finite-rate chemistry have been proposed in Refs. [16,17]. Other approaches for autoignition in the presence of turbulence include models based on transport equations for flame surface density [18–20] and transported PDF methods [21,22], both of which give overall good predictions.

Alternative modeling based on conditional moment closure has been proposed in Refs. [23,24]. Successful use of CMC for autoignition problems in simplified flow fields with both first- [25] and second-order [26] closure of the chemical source term has been reported, whereas its applicability to spray autoignition with first-order closure has also been shown [27,28]. In principle, a proper account of turbulence–chemistry interactions throughout the autoignition phase needs to include fluctuations of the scalar dissipation rate [29,30], as in second-order CMC [26]. In practice, however, the computationally simpler first-order closure must be explored for engine calculations before the added complexity and cost of the second-order approach are justified.

This investigation revisits the spray autoignition problem treated by Kim and Huh [27]. The aim is to explore in more detail the need for a fully elliptic CMC formulation, and, because of the availability of refined experimental data in a diesel-like environment [31], to validate numerical methods for the mul-