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Constant volume n-Heptane autoignition using One-Dimensional Turbulence

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ABSTRACT

Constant volume premixed lean n-Heptane/air autoignition at high pressure is investigated using the One-Dimensional Turbulence (ODT) model. The configuration consists of a 1D fixed volume domain with a prescribed velocity spectrum and temperature fluctuations superimposed on an initial uniformly elevated scalar field. The sensitivity of the heat release rate and pressure evolution to the initial temperature distribution is studied by imposing different initial temperature fields while holding the mean, RMS and integral length scale of the field constant. Three detailed chemical mechanisms are employed for the prediction of autoignition and heat release rate. To mitigate the high computational cost associated with the calculation of the chemical source terms in the stiff complex mechanisms, an approach based on the Strang-Splitting method is presented. Finally, a study of the ODT model uncertainty is carried out. For validation, ODT results are compared to 2D DNS data from Yoo et al. (2011) for the temporal evolution of heat release rate, pressure and density-weighted displacement speed. Ensemble averaged ODT results show good agreement with the DNS data. ODT results generated from varying the initial temperature fields show that the ignition delay time is highly sensitive to the initial temperature field. The ODT model uncertainty study shows that dispersion due to the stochastic nature of the model is considerably smaller than the dispersion resulting from varying the initial temperature field. Overall, this study demonstrates that ODT accurately captures the evolution of complex chemistry reactive flows in constant volume autoignition simulations and that once validated, ODT is an efficient tool that can be used to carry out parametric studies not feasible by DNS.

1. Introduction

The volumetric energy density of fossil fuels in the energy transport sector has led to their dominance over emerging, alternative fuels in the field. Among the different types of fossil fuels, the characterization of n-Heptane as a surrogate fuel for Diesel takes strategic importance, mainly due to the wide range of operational conditions over which it can be used. In this context, there has been a significant amount of time and effort in combustion research devoted to the topic of Homogeneous Charge Compression Ignition (HCCI) engines. HCCI engines have shown that very low emissions and high fuel efficiency values are feasible through constant volume autoignition.

Several Direct Numerical Simulation (DNS) studies have been focused on the topic of constant volume autoignition [1–7]. Within the DNS research, the study of constant volume autoignition has led not only to the understanding of interesting fundamental phenomena, well detailed in the work of Yoo et al. [5], but it has also symbolized the achievement of major milestones in terms of computational power. A pioneering 2D DNS that considered inhomogeneous scalar fields was performed with reduced hydrogen/air chemistry by Sankaran et al. [4], and a follow-up study with a wider range of initial conditions was carried out by Chen et al. [2]. The latter study allowed a clearer characterization of deflagration and detonation regimes during constant volume autoignition processes. The study was also chosen as a test case for the Linear Eddy Modeling (LEM) approach in constant volume autoignition, discussed by Oevermann et al. [8].

It was not, however, until 2011 that increased computational power and a series of chemistry reduction methods allowed the first 2D DNS simulation for a n-Heptane/air mixture by Yoo et al. [5]. This work showed that RMS temperature fluctuations have a first-order effect on the ignition characteristics of n-Heptane/air

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mixtures. In 2013, another milestone was achieved by Yu and Bai [6], who conducted the first 3-D DNS of a constant volume autoignition environment with a premixed hydrogen/air gas mixture. The work by Yu and Bai [6] is pioneering in the sense that a first insight was given to the turbulence dynamics within autoignition, e.g. by studying the Turbulent Kinetic Energy (TKE) evolution prior to ignition.

Despite the robustness of the LEM results [8] previously cited, the findings in [6] show the importance of the evolution of the turbulent state of the flow on the ignition characteristics. Such influences cannot be obtained in LEM due to the inherent limitations of the model. This is the reason why the One-Dimensional Turbulence (ODT) model gains importance in this case.

In essence, as a stand-alone model, ODT belongs to the family of stochastic turbulence models. ODT does not model small scale phenomena, but as in DNS, it is directly resolved. In contrast to DNS, however, 3-D Navier–Stokes turbulence is modeled via a solution dependent sequence of stochastic 1-D events. ODT preserves many characteristics of LEM, but additionally features an intrinsic dynamic feedback between the turbulent fluctuations and the average state of the flow [9].

Recent ODT studies followed DNS research by gradually increasing the complexity of the benchmark cases. Jozefik et al. [10] considered a variable density formulation for ODT in a constant volume autoignition process as a benchmark test for the introduction of the Darrieus–Landau instability model. Building upon this, the compressible ODT formulation in [11] followed. For an application-relevant fuel like n-Heptane, the computational savings of ODT in comparison to DNS could allow important insights regarding the behavior of the fuel in complex operating conditions such as constant volume autoignition processes. With this work, the authors present the first framework for the treatment of stiff chemistry for such processes within ODT. As a stepping stone from the previous LEM study, this work is also focused on the influence of temperature inhomogeneities in the initial highly reactive mixture.

This paper is organized as follows. Section 2 provides the modeling approach. Specifically, Section 2.1 presents the numerical formulation, Section 2.2 gives a short overview of ODT, Section 2.3 introduces the ODT constant volume configuration specific models, Section 2.4 describes the Strang-Splitting method and the numerical time advancement, and Section 2.5 discusses the mesh adaption procedure. In Section 3, details concerning the configuration are given and in Section 4, ODT results are compared to DNS data for the temporal evolution of heat release rate, pressure and density-weighted displacement speed. These results are discussed from the point of view of the influence of randomized initial conditions in Section 4.1, the sensitivity to the ODT model parameters in Section 4.2, and the influence of the magnitude of the temperature inhomogeneities in Section 4.3. The sensitivity of the simulations to the initial conditions is also compared to the uncertainty of the ODT model (due to the 1-D stochastic events). An additional sensitivity analysis linked to the reaction chemistry is also presented. Concluding remarks are provided in Section 5. In Appendix A, details of the velocity evolution in ODT are given and in Appendix B, a convergence analysis of the time-stepping scheme is shown.

2. ODT model formulation

2.1. Conservation equations for the diffusion–reaction system

Due to the one-dimensional modeling of multi-dimensional turbulence interactions in ODT, the generalized Navier–Stokes equations are not solved by the model. Rather, a set of diffusion–reaction evolution equations coupled to instantaneous implementation of stochastic 1-D eddy events is considered. The main idea behind the ODT modeling is the separate treatment of the diffusion/reaction processes from the turbulent advection. As such, the structure of the theoretical and modeling background in this paper will also separately address these two components of ODT.

Although previous work done by Jozefik et al. [11] introduced a compressible formulation for ODT, the stiffness of the chemistry employed in this study forced the authors to opt for the simpler Zero-Mach classical ODT formulation, which has been the subject of numerous publications in the field of reactive flows (see e.g. [12–14]). In terms of comparison to the DNS from Yoo et al. [5], only relatively large values of initial RMS temperature fluctuations are evaluated in this paper. According to Yoo et al. [5], these large initial RMS temperature fluctuations values translate into deflagration-dominated regimes with a characteristic low subsonic displacement speed. This guarantees the validity of the Zero-Mach limit approximation.

The details of the diffusion–reaction evolution equations are given here considering a Lagrangian formulation of the conservation equations, similar to the framework in [15]. The conservation of properties in each of the control volumes in the one-dimensional domain is given by the application of the Reynolds Transport Theorem (RTT) to a Lagrangian system intensive property β,

$$\frac{d}{dt}\int_{\forall_{(t)}} \rho\beta d\forall = \frac{\partial}{\partial t}\int_{CV} \rho\beta d\forall + \oint_{CS} \rho\beta(\vec{V}-\vec{V}_{CV})\cdot d\vec{S}. \tag{1}$$

In Eq. (1), CS refers to the boundary of the Control Volume (CV), ρ is the density of the Lagrangian system and $\forall$ represents the Lagrangian system volume. If the velocities of the equivalent moving CV are assumed to be equal to the Lagrangian system velocities, $\vec{V}_{CV} = \vec{V} = u_{L,j}$, then it is possible to omit the last term on the Right-Hand Side (RHS) of Eq. (1). We use $u_{L,j}$ to refer to the three components of the Lagrangian system velocity. These are not equivalent to the three velocity components normally solved in ODT, u_j. Details of the relation between the ODT velocity components u_j and the Lagrangian velocities $u_{L,j}$, which comply with Eq. (1), can be found in Section 2.3.

In the Zero-Mach number limit combustion, the velocity field admits an orthogonal decomposition into zero-divergence and non-zero-divergence contributions [16]. Similar considerations can be applied to the diffusion–reaction evolution of the Lagrangian velocity field considered here. We define our system of equations for Zero-Mach combustion as one comprised by the variables of thermodynamic pressure P, the Lagrangian velocity field $u_{L,j}$, the species mass fractions present in the gas mixture Y_k and the enthalpy of the mixture h. Such a system of equations, in terms of non-conservative variables, implies conservation of mass, i.e. the density evolution Partial Differential Equation (PDE) can be derived from such a system of equations, although it does not need to be resolved directly [16]. The system of equations comprises then a PDE for momentum conservation acting over a zero-divergence velocity contribution for $u_{L,j}$, species mass fractions and enthalpy PDEs, an expression for the temporal rate of change of the pressure, as well as the non-zero divergence condition for the complementary contribution to $u_{L,j}$.

The momentum equation evolution is used in ODT as a mechanism to update the velocity components influencing the selection of eddy events, i.e., the ODT velocity components u_j experiencing diffusion evolution and influencing turbulent advection (see Section 2.2). u_j velocity components comprise the divergence-free part of $u_{L,j}$. The formulation for the momentum equation in this work follows then the original incompressible ODT momentum evolution in [15], derived from the RTT, Eq. (1),

$$\rho\frac{\partial u_j}{\partial t} = \frac{\partial}{\partial x}\left(\mu\frac{\partial u_j}{\partial x}\right), \tag{2}$$