Combustion and Flame 178 (2017) 70–81

Contents lists available at ScienceDirect

Combustion and Flame

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

Turbulence effects on the autoignition of DME in a turbulent co-flowing jet

Tarek Echekki [a,*], Samer F. Ahmed [b]

[a] Department of Mechanical and Aerospace Engineering, Campus Box 7910, North Carolina State University, Raleigh 27695, NC, USA
[b] Thermofluids Group, Department of Mechanical and Industrial Engineering, College of Engineering, Qatar University, P.O. Box 2713, Doha, Qatar

ARTICLE INFO

Article history:
Received 1 September 2016
Revised 12 October 2016
Accepted 20 December 2016
Available online 5 February 2017

Keywords:
Turbulent jet ignition
The one-dimensional turbulence model
Autoignition
DME fuel

ABSTRACT

Dimethyl ether (DME) autoignition in turbulent co-flowing jets with preheated air is studied using the one-dimensional turbulence (ODT) model. We investigate the effects of molecular and turbulent transport on the autoignition process at different jet Reynolds numbers and two air preheat conditions. Statistics for the cases considered show that the overall effects of turbulence and molecular transport can serve to delay or accelerate autoignition depending upon where ignition starts, the presence of 2-stage or single-stage ignition and the variations in ignition delay times in mixture fraction space. For the higher temperature air preheat cases, the classical view that autoignition is delayed by turbulence is established. For the lower preheat air temperature cases, we show that low-temperature chemistry associated with first-stage ignition can help accelerate the autoignition process and the transition to high-temperature chemistry. This acceleration can reduce the ignition delay time by as much as a factor of 2. Given this work and previous work by the authors based on a different fuel, n-heptane, we find that the ignition delay map based on homogeneous ignition for different mixture fractions can provide a preview of the ignition scenarios for the co-flowing jet configuration regardless of the choice of fuel considered.

1. Introduction

Many practical combustion fuels exhibit multi-stage ignition associated with the so-called negative temperature coefficient (NTC) behavior. This behavior introduces additional key chemical time scales associated with the different stages of ignition. This behavior is critical for a broad range of practical fuels; yet, we are only beginning to understand various scenarios where NTC behavior coupled with chemistry can exhibit unexpected results. It has been commonly assumed that turbulence serves to delay ignition because of the inherent role of dissipation in depleting nascent flame kernels of key radicals and heat [1–8]. However, recent studies suggest that the coupling of reaction and transport (turbulent or molecular) can yield complex interactions that may or may not fall into the common view of the role of turbulent transport (see for example, [9–14]).

In a recent study, the authors investigated the coupling of chemistry and transport in a jet configuration of n-heptane, a fuel subject to NTC behavior, in preheated co-flow air at various jet Reynolds numbers [14] using the one-dimensional turbulence (ODT) model [15]. We have observed a mechanism by which turbulent and molecular transport can accelerate the autoignition process through transport from layers in the fluid experiencing first-stage ignition to layers evolving eventually to their second- or final-stage ignition. However, this mechanism is only one possible scenario where transport can potentially accelerate ignition under turbulence conditions. More importantly, ignition delay maps relating ignition delay for first and second stage ignitions vs. mixture fraction based on homogeneous ignition helped explain the trends exhibited in the jet simulations.

The coupling of first-stage and second-stage chemistries has been identified by other authors within the context of non-premixed flame stabilization [16–19] and related to the fuel being considered in this study, which is dimethyl ether (DME). For example, Deng et al. [16] showed that at an intermediate temperature range for the co-flow air in a stabilized non-premixed DME/air jet flame, NTC chemistry determines the stabilization point in mixture fraction space. Minomoto and Chen [19] also show that the propagation speed at the triple point of a stabilized DME/air slot jet flame is also influenced by two-stage ignition.

The objective of this study is to explore and identify additional scenarios exhibited by fuels subject to NTC behavior under turbulence conditions. More importantly, we attempt to preview such scenarios using ignition delay maps based on homogeneous ignition calculations. The study is based on the ODT

* Corresponding author.
E-mail address: techekk@ncsu.edu (T. Echekki).

http://dx.doi.org/10.1016/j.combustflame.2016.12.022
0010-2180/

model applied to DME, a relatively simple fuel to heavier hydrocarbons that exhibits NTC behavior, in a co-flowing jet configuration. To overcome potential limitations of reduced mechanisms for complex fuels, which are validated for simple reactor models, we will use the detailed mechanism proposed by Zhao et al. [20]. This mechanism captures both low-temperature and high-temperature kinetics for DME. There are several detailed mechanisms for DME, which are available in the literature [21–26]. The mechanism by Zhao et al. [20] has been validated against a host of experiments spanning the low- and high-temperature regimes in combustion, including experiments based on flow reactors, shock tubes, jet-stirred reactors and burner-stabilized premixed flames [20]. In the present study, to further characterize the NTC behavior, we also carry out 0D simulations.

2. Model formulations and run conditions

Two types of simulations are implemented, which include: 1) zero-dimensional homogeneous reaction ignition, and 2) one-dimensional stochastic model that emulates combustion in a jet configuration. The two models are described below.

2.1. 0D simulations

The zero-dimensional simulations serve as references for autoignition studies in the presence of turbulence and molecular transport. The governing equations for a zero-dimensional constant pressure system comprised of N chemical species correspond to the species and the temperature equations:

- The species equation:

$$\frac{\partial Y_k}{\partial t} = \frac{\dot{\omega}_k}{\rho}. \tag{1}$$

- The temperature equation:

$$\frac{\partial T}{\partial t} = -\frac{1}{\rho \bar{c}_p} \sum_{k=1}^{N} h_k \dot{\omega}_k. \tag{2}$$

In the above equations, t is the independent variable, which corresponds to time; T is the temperature; Y_k is the kth species mass fraction; ρ is the mixture density; $\dot{\omega}_k$ is the kth species reaction rates; $\bar{c}_p$ is the mixture specific heat; and h_k is the kth species total enthalpy. The thermodynamic pressure, p, is assumed to be constant, and the equation of state:

$$\rho = \frac{p}{R_u T \sum_{k=1}^{N} (Y_k/W_k)}, \tag{3}$$

can be used to determine the mixture density. The governing equations are integrated using a modified version of the CHEMKIN II code SENKIN [27].

The solution usually starts with an initial homogeneous mixture of fuel and oxidizer at different equivalence ratios from lean to rich. By varying the mixture fraction, different fuel and preheated oxidizer compositions are obtained. These initial compositions of the mixture based on the prescribed mixture fraction, Z, are prescribed as follows:

$$Y_{\text{Fuel}} = Z, \; Y_{\text{Oxidizer}} = 1 - Z. \tag{4}$$

The corresponding mixture temperature, T_{mix}, is evaluated by adiabatic mixing of the preheated air with the fuel at the prescribed mixture fraction:

$$\begin{aligned} &Z \times h_{\text{Fuel}}(T_{\text{Fuel}}) + (1-Z) \times h_{\text{Oxidizer}}(T_{\text{Oxidizer}}) \\ &\quad = Z \times h_{\text{Fuel}}(T_{\text{mix}}) + (1-Z) \times h_{\text{Oxidizer}}(T_{\text{mix}}) \end{aligned} \tag{5}$$

The scope of the homogeneous ignition study is to identify the various ignition scenarios at different mixture fractions and to provide a reference case for comparison with jet autoignition.

2.2. ODT simulations

A detailed description of the ODT model formulation for the jet configuration is given by Echekki et al. [15]. The ODT model is based on a deterministic implementation of reaction and diffusion and a stochastic implementation of turbulent advection in a space- and time-resolved simulation on a 1D domain. In this problem, the 1D domain corresponds to the transverse direction of the mean flow. Therefore, the formulation is based on a planar temporally-developing jet configuration. The formulation is built on the two key assumptions: (1) a parabolic flow formulation where transverse processes are dominant and streamwise downstream processes are less important, and (2) the time scales governed by the shear (in the transverse direction) are representative of the time scales representing stirring process in the jet. Moreover, as indicated in Echekki et al. [15], there are inherently similar scaling relations for the velocity decay between a planar temporally-developing jet (as implemented here) and the spatially-developing round jet.

Molecular processes are prescribed by the following unsteady reaction-diffusion equations:

- The streamwise momentum equation:

$$\frac{\partial u}{\partial t} = \frac{1}{\rho} \frac{\partial}{\partial y} \left(\mu \frac{\partial u}{\partial y} \right). \tag{6}$$

- The species equation:

$$\frac{\partial Y_k}{\partial t} = -\frac{1}{\rho} \frac{\partial}{\partial y} (\rho V_k Y_k) + \frac{\dot{\omega}_k}{\rho}. \tag{7}$$

- The temperature equation:

$$\frac{\partial T}{\partial t} = \frac{1}{\rho \bar{c}_p} \sum_{k=1}^{N} c_{p,k} Y_k V_k \frac{\partial T}{\partial y} + \frac{1}{\rho \bar{c}_p} \frac{\partial}{\partial y} \left(\lambda \frac{\partial T}{\partial y} \right) - \frac{1}{\rho \bar{c}_p} \sum_{k=1}^{N} h_k \dot{\omega}_k. \tag{8}$$

The pressure is assumed to be spatially uniform and constant, and the equation of state (3) is used to determine the mixture mass density. $c_{p,k}$ and V_k represent the kth species specific heat and diffusion velocity, respectively; λ is the mixture thermal conductivity. Eqs. (6)–(8) represent a temporal solution of a turbulent jet flame. The temporal evolution may be interpreted, in a statistical sense, as a downstream spatial evolution (in x) of the 1D velocity and scalar profiles. However, this conversion is not implemented here and statistics are collected as a function of time to establish direct comparisons with the unsteady 0D simulations. Therefore, the simulations are implemented as temporal jet simulations for one principal reason: the progress in the autoignition process in a temporal jet can be compared directly to the homogeneous ignition results. Such comparisons, will enable an isolation of turbulent transport and molecular diffusion transport effects on the autoignition process. A direct conversion from temporal to spatial jet statistics can be carried out in principle by accounting for residence time effects associated with the different inlet velocities at the co-flowing streams.

In the jet simulations, turbulent advection is implemented stochastically using stirring events, each involving the application of a “triplet map” [15]. The frequency of stirring events is governed by the spatially-resolved evolving rate of shear in the jet. Two adjustable parameters, the so-called A and β [15], are identical to previous values used in jet configurations with ODT [14,28–32].

The initial configuration (also, corresponding to the jet inlet) consists of a 2D segregated central fuel jet of width 1.1 cm with preheated air in the co-flow. The spatial extent of the co-flow air depends primarily on the evolution of the jet and the Reynolds number resulting in computational domains of 16 cm to 24 cm