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Autoignition of n-heptane in a turbulent co-flowing jet

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ABSTRACT

N-heptane autoignition in turbulent co-flowing jets with preheated air is studied using the one-dimensional turbulence (ODT) model. The simulations are designed to investigate the effects of molecular and turbulent transports on the process of autoignition. Both homogeneous and jet configuration simulations are carried out. The jet configurations are implemented at different jet inlet Reynolds numbers and for two air preheat conditions. Statistics for the cases considered show that, while the onset of autoignition may be delayed by turbulence, the eventual evolution of the volumetric heat release rate indicates that turbulence enhances the post-ignition stages. Since different regions of the mixture can have different ignition delays and may be characterized by one- or two-stage ignition, the autoignition process can be accelerated by ignition kernel propagation or the role of heat dissipation may be reduced through the prevalence of one-stage and two-stage ignitions in different regions of the mixture.

1. Introduction

Autoignition is an important process for initiating or sustaining combustion in a number of practical devices [1,2]. It is also considered a viable mechanism for flame stabilization in non-premixed systems when either or both the fuel or oxidizer streams are preheated to ignition temperatures [3]. Conditions of ignition are governed by the competition of ignition chemistry with molecular and turbulent transport; and this competition may determine the fate or intensity of the combustion process. In igniting mixtures, this competition also determines the autoignition delay time and the associated lift-off height.

In addition to fuel autoignition in vitiated coflow [3], fuel autoignition in preheated coflow air [4,5] represents a useful canonical problem for autoignition that is relevant to practical problems. This configuration has been the subject of a number of experimental and numerical studies, including the more recent work of Echekki and Gupta [6,7], with a limited range of fuels, including hydrogen and syngas. A number of control parameters are found to play an important role in the autoignition process, including the fuel composition, the preheat temperature of the oxidizer, and the inlet conditions (mean flow and turbulence). Flow inlet conditions are associated with the role of the evolving scalar dissipation rate field on autoignition delay. For example, Markides and Mastorakos [4] find that turbulence serves to delay the autoignition process for hydrogen fuels. Similar trends are found in other studies as well, including a more recent study by Echekki and Gupta [6].

The roles of turbulence and the evolving scalar dissipation field reflect a relatively complex picture of the competition between transport (molecular and turbulent) and chemistry. An earlier study by Mastorkas et al. [8] has shown that autoignition in non-homogeneous mixtures is initiated at variable mixture conditions (composition and temperature) and low rates of dissipation. This observation was further corroborated by subsequent studies with complex chemistry, including the more recent work by Im and Chen [9], Hilbert and Thévenin [10] and Echekki and Chen [11]. Turbulent transport, in addition to the presence of the shear layer separating the fuel and the co-flow, result in the presence of scalar dissipation, which depletes radicals and heat from nascent ignition kernels [11]. Turbulence can serve to modulate the scalar dissipation by either increasing the rate of scalar dissipation or reducing it, as the fuel and oxidizer streams mix.

In this paper, we investigate numerically turbulent jet autoignition using a reduced mechanism for n-heptane using the one-dimensional turbulence (ODT) model [12]. The ODT approach, which is based on 1D unsteady simulations with a stochastic implementation for turbulent transport and a deterministic implementation for the coupling of chemistry and molecular transport, has already been implemented for the study of jet autoignition in hydrogen and hydrogen/carbon monoxide fuels [6,7].

The model represents a valid formulation for jet flames stabilized by autoignition where an inherently parabolic formulation can be adopted. The formulation assumes that downstream effects, especially those responsible for upstream propagation and flame

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stabilization, do not influence the onset of autoignition or the stabilization mechanism for the jet diffusion flames. It is expected to be valid for a class of lifted flames where the dominant stabilization mechanism is based on autoignition. The study highlights the key roles of molecular and turbulent transport in large hydrocarbon autoignition in a turbulent jet configuration.

N-heptane is an important primary reference fuel for gasoline and diesel fuels. An important feature of n-heptane ignition is the presence of the so-called negative temperature coefficient (NTC). The NTC behavior under certain conditions also results in 2-stage ignition where the temperature initially rises, then, the mixture undergoes a phase of endothermic reactions before the temperature rises again. Within the context of turbulent autoignition, two-stage ignition introduces additional time scales where turbulent and molecular transports can play a role in delaying or enhancing the autoignition process.

2. Model formulations and run conditions

Two sets of simulations are carried out using the 58-species reduced mechanism for n-heptane by Yoo et al. [13]. The mechanism was developed with a two-stage directed relation graph (DRG) approach starting from the LLNL detailed mechanism for n-heptane with 561 species and 2539 reactions [14]. The mechanism was validated using different combustion applications, including ignition, extinction, premixed flame structure and propagation.

The two sets of simulations include:

1. Zero-dimensional homogeneous reaction solver, and
2. One-dimensional stochastic model that emulates combustion in a jet configuration.

The two models are described below.

2.1. Zero-dimensional models

The zero-dimensional simulations for homogeneous ignition are used partly (1) to characterize the autoignition process of n-heptane fuel as a function of mixture fraction given prescribed oxidizer preheat and pre-vaporized fuel temperatures, (2) to identify the most favorable mixture conditions for autoignition and (3) to provide a reference case for comparison with jet autoignition under molecular and turbulent transports.

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, all the symbols have their usual meaning. 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 (in dimensions of mass per unit volume per unit time); $\bar{c}_p$ is the mixture specific heat; and h_k is the kth species total enthalpy (combining both chemical and sensible enthalpies). 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 [15]. The system is integrated using a variant of the DASSL software called DASAC [16].

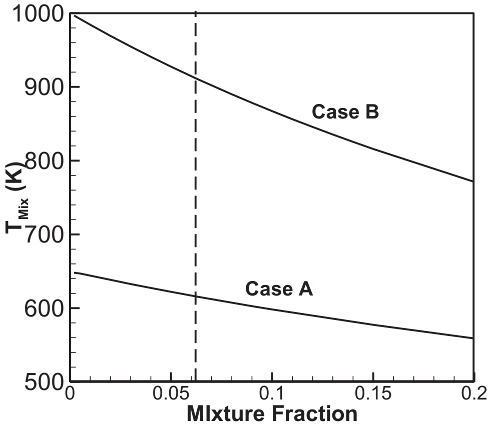

Fig. 1. Initial mixture temperature based on the prescribed mixture fraction for cases A and B. The stoichiometric condition is shown with the dashed line.

The simulations are designed to complement the jet studies, which prescribe unique temperatures for the oxidizer and the fuel. A range of mixture fractions are considered where the fuel and oxidizer are mixed adiabatically at fixed pressure (i.e. constant enthalpy) to yield a mixture composition and temperature. Given that the oxidizer is preheated, the fuel-lean conditions (i.e. low mixture fractions) have higher temperatures then the fuel-rich conditions.

In these studies we have prescribed the fuel and oxidizer temperatures, T_{fuel} and T_{oxid}, and varied the mixture composition from fuel-lean to fuel-rich by prescribing a mixture fraction (0 for all oxidizer, 1 for all fuel), Z. The initial mass fraction for a given kth species in the mixture for a given mixture fraction is prescribed based on its composition in the fuel and the oxidizer and the mixture fraction as follows:

$$Y_k = Z \times Y_{k,\text{Fuel}} + (1 - Z) \times Y_{k,\text{Oxidizer}} \tag{4}$$

where the subscripts “Fuel” and “Oxidizer” refer to the mass fractions of the kth species in the fuel and the oxidizer streams, respectively. The mixture temperature, T_{mix}, is prescribed by solving the solutions for adiabatic mixing:

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

The mixture conditions corresponding to this study correspond to a reference state of pre-vaporized fuel at 400 K and 1 atm and two different air preheat temperatures at 650 K, identified as case A, and 1000 K, identified as case B, both at atmospheric pressures.

The run conditions were selected around the stoichiometric mixture fraction of 0.0621 and range for values of the mixture fraction from 0.002 to 0.2. Figure 1 shows the initial mixture temperatures for both cases A and B based on the values of the mixture fractions considered. Because of the differences between the specific heats of the fuel and the oxidizer species, the initial mixture temperature profiles are not linear in mixture fraction space.

2.2. One-dimensional turbulence (ODT) model

Practical configurations of combustion of n-heptane fuel invariably require combustion in a turbulent environment. We are using a very powerful and relatively low-computational cost tool to advance our understanding of autoignition in turbulent media. The tool is based on simulations using the stand-alone one-dimensional turbulence (ODT) approach. A detailed description of the ODT model formulation for the jet configuration is given by Echekki et al. [12].