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Proceedings of the Combustion Institute 000 (2016) 1–8

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Proceedings
of the
Combustion
Institute

Effects of initial temperature on autoignition and detonation development in dimethyl ether/air mixtures with temperature gradient

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Received 2 December 2015; accepted 3 August 2016

Available online xxx

Abstract

For large hydrocarbon fuels used in internal combustion engines, different low-temperature and high-temperature chemistries are involved in the autoignition processes under different initial temperatures. As one of the simplest fuels with low-temperature chemistry, dimethyl ether (DME) is considered in this study and one-dimensional autoignitive reaction front propagation induced by temperature gradient is simulated for stoichiometric DME/air mixtures considering detailed chemistry and transport. The emphasis is placed on assessing and interpreting the influence of initial temperature on the detonation development regime. Different initial temperatures below, within and above the negative-temperature coefficient (NTC) region are considered. For each initial temperature, four typical autoignition modes are identified: supersonic autoignitive reaction front (without detonation); detonation development; transonic reaction front; and subsonic reaction front. The detonation development regimes for two fuels, DME and n-heptane, at the same initial temperature and those for the same fuel, DME, at three different initial temperatures respectively below, within and above the NTC region are obtained. Based on these results, the influence of fuel type and initial temperature on detonation development regime are discussed. It is found that the detonation development regime becomes narrower at higher initial temperature. Moreover, the influence of initial temperature on reaction front propagation speed is investigated. The reaction front propagation speed is shown to be strongly affected by different chemistries involved in low and high temperature regions. When only the high-temperature chemistry is involved, the reaction front propagation speed is shown to be less dependent on the initial temperature.

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Keywords: Autoignition; Detonation; Temperature gradient; Dimethyl ether

1. Introduction

Autoignitive reaction front propagation in mixtures with temperature inhomogeneity may occur

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<http://dx.doi.org/10.1016/j.proci.2016.08.014>

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in traditional spark ignition engines (SIEs) and advanced internal combustion engines such as HCCI and SACI engines [1–4]. During such autoignitive reaction front propagation, detonation development happens under certain conditions and it can cause engine knock in SIEs [1,2]. Moreover, such kind of autoignition may cause difficulties in the control of ignition timing in HCCI and SACI engines [3,4]. Therefore, autoignition in mixtures with temperature non-uniformity has received great attention recently (e.g., [5] and references therein).

Zel'dovich [6] first developed the theory on autoignitive reaction front propagation caused by reactivity non-uniformity. It was proposed that different modes of reaction front propagation can be induced by the gradient of ignition delay time and that detonation can develop at certain conditions [6]. The theory of Zel'dovich was verified and extended by many researchers (e.g., [7–11]). Among them, Bradley and coworkers [8,9] investigated different modes of reaction front propagation from a hot spot in syngas/air mixtures using one-dimensional simulation. They studied the critical conditions for detonation development and proposed an operational peninsula within which detonation can develop from temperature inhomogeneity. The detonation peninsula was then used by Bradley and Kalghatgi [2,12,13] in the study of engine knock. It was demonstrated that the detonation peninsula helps to determine the critical conditions for detonation development in engines and thereby it is a very useful tool in the study of engine knock [2,13–16].

Though it was determined only for syngas [8,9], the detonation peninsula was used for different hydrocarbon fuels [2,12,13]. It has not been checked whether this detonation peninsula also works for other fuels besides syngas. Rudloff et al. [14] first suggested the dependence of detonation development regime on fuel and they proposed to conduct simulations for other fuels [8]. Therefore, there is a need to investigate the detonation development regime for fuels other than syngas.

Unlike syngas, large hydrocarbon fuels used in engines usually have complicated low-temperature chemistry and negative-temperature coefficient (NTC) phenomenon. Therefore, at different initial temperatures below, within and above the NTC region, the detonation development regime and autoignitive reaction front propagation behavior may be different. In the literature, direct numerical simulations of autoignition in mixtures with thermal stratification were conducted for several fuels with low-temperature chemistry, e.g., dimethyl ether (DME) [17], n-heptane [18] and iso-octane [4,19]. However, in these studies detonation development was not investigated. Zhang et al. [20] examined the coupling effects of concentration and temperature gradients on autoignition modes and proposed a general critical boundary to separate the spontaneous ignition mode from detonation modes

in the two dimensional concentration and temperature gradient phase space. In our recent work [21,22], the temperature gradient-induced autoignitive reaction front propagation in n-heptane/air mixture was investigated. It was found that the low-temperature chemistry results in complicated reaction-pressure wave interactions. Therefore, it is of interest to further study how the initial temperature affects detonation development regime and autoignitive reaction front propagation for fuels with low-temperature chemistry. Since DME is one of the simplest fuels with low-temperature chemistry, it is studied in the present work.

Based on the above considerations, the objectives of this study are to obtain the detonation development regimes for fuels other than syngas and to examine the effects of initial temperature on autoignitive reaction front propagation and detonation development regime. Unlike our previous studies [21,22] which mainly considered planar geometry, this study focuses on spherical geometry (same as that of Bradley and coworkers [9] and similar to hot/cold spots in engines). Therefore, the detonation development regimes obtained here can be compared with that in [9] for syngas. Furthermore, for the same fuel, DME, the detonation development regimes at different initial temperatures below, within and above the NTC region are obtained and compared in this study.

2. Numerical model and specifications

The present model is the same as that of Bradley and coworkers [9]. We consider the autoignitive reaction front propagation from a hot or cold spot at the center of a closed spherical chamber. The initial temperature distribution is

$$T(t = 0, r) = \begin{cases} T_0 + (r - r_0) \frac{dT_0}{dr} & \text{for } 0 \leq r \leq r_0 \\ T_0 & \text{for } r_0 \leq r \leq R_W \end{cases} \quad (1)$$

where t and r are respectively the temporal and spatial coordinates; r_0 is the size of hot/cold spot; $R_W = 10$ cm is the radius of the spherical chamber; dT_0/dr is the temperature gradient to be specified ($dT_0/dr < 0$ for hot spot and $dT_0/dr > 0$ for cold spot); and T_0 is the initial temperature of the mixture outside of the hot/cold spot. The whole computational domain is initially filled with static fuel/air mixture at the pressure of $P_0 = 40$ atm. We limit our focus to laminar combustion and thereby the initial flow is static without turbulence. At both boundaries (i.e., $r = 0$ and $r = R_W$), zero flow speed and zero gradients of temperature and mass fractions are enforced.

The transient autoignition process is simulated using the in-house code A-SURF. The conservation equations for one-dimensional, compressible,

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