

available at www.sciencedirect.comwww.elsevier.com/locate/fuproc

Dimethyl ether autoignition in a rapid compression machine: Experiments and chemical kinetic modeling

Gaurav Mittal^a, Marcos Chaos^{b,*}, Chih-Jen Sung^a, Frederick L. Dryer^b

^aDepartment of Mechanical and Aerospace Engineering, Case Western Reserve University, Cleveland, OH 44106, USA

^bDepartment of Mechanical and Aerospace Engineering, Princeton University, Princeton, NJ 08544, USA

ARTICLE INFO

Article history:

Received 15 February 2008

Received in revised form 27 May 2008

Accepted 29 May 2008

Keywords:

Dimethyl ether

Ignition

Rapid compression

Chemical kinetics

Induction chemistry

ABSTRACT

Dimethyl ether (DME) autoignition at elevated pressures and relatively low temperatures is experimentally investigated using a rapid compression machine (RCM). DME/O₂/N₂ homogeneous mixtures are studied over an equivalence ratio range of 0.43–1.5 and at compressed pressures ranging from 10 to 20 bar and compressed temperatures from 615 to 735 K. At these conditions RCM results show the well-known two-stage ignition characteristics of DME and the negative temperature coefficient (NTC) region is noted to become more prominent at lower pressures and for oxygen lean mixtures. Furthermore, the first-stage ignition delay is found to be insensitive to changes in pressure and equivalence ratio. To help interpret the experimental results, chemical kinetic simulations of the ignition process are carried out using available detailed kinetic models and, in general, good agreement is obtained when using the model of Zhao et al. [Int. J. Chem. Kinet. 40, 2008, 1–18]. Sensitivity analyses are carried out to help identify important reactions. Lastly, while it is implicitly assumed in many rapid compression studies that chemical changes from the initial charge conditions that might occur during compression are negligible, it is herein shown with the help of Computational Singular Perturbation (CSP) analyses that chemical species formed during compression with little evolved exothermicity can considerably affect autoignition observations. Therefore, it is essential to simulate both compression and post-compression processes occurring in the RCM experiment, in order to properly interpret RCM ignition delay results.

© 2008 Elsevier B.V. All rights reserved.

1. Introduction

Environmental pollution, energy security, and future oil supplies are concerns that have driven the global community to seek nonpetroleum-based alternative fuels, along with more advanced energy technologies to increase the efficiency of energy use. Dimethyl ether (DME) appears to have a large potential as an energy source. DME has been proposed as a promising alternative to diesel fuels due to its high cetane number [1]. In recent years DME has emerged as a fuel additive to reduce particulate and NO_x emissions due to its overall low

sooting and polluting potentials. DME can be mass-produced from extensive feedstocks, including natural gas, coal, and biomass; its physical properties are similar to those of Liquefied Petroleum Gases (LPG), so DME can be stored and distributed using established LPG infrastructures [2,3]. In addition, DME can also be used as an ignition enhancer in propulsion systems and internal combustion engines [4,5].

Autoignition of engine-relevant fuels, such as DME, at practical conditions (i.e. high pressures and intermediate to low temperatures) is of fundamental importance to emerging technologies such as Homogeneous Charge Compression

* Corresponding author. Department of Mechanical and Aerospace Engineering, Princeton University, Princeton, New Jersey 08544-5263, USA. Tel.: +1 609 258 2947; fax: +1 609 258 6109.

E-mail address: mchaos@princeton.edu (M. Chaos).

Ignition (HCCI) [6]. Furthermore, interest and advancements in fuel-flexible gas turbine power generation systems that use DME [7] require the knowledge of its ignition and burning characteristics. DME shock tube ignition studies are available in the literature [8–11]; however, with the exception of the studies of Pffhal et al. [8] and Zinner and Petersen [11], few DME ignition results are available at pressure and temperature conditions of practical interest.

In kinetic research, several detailed chemical models for low and high temperature DME oxidation [12–17] have been developed and validated against multiple experimental observations. Of particular importance to the present study is the ability of available chemical kinetic models to accurately reproduce DME autoignition properties at engine-like conditions. DME displays the classical two-stage, negative temperature coefficient (NTC) ignition behavior similar to that observed with linear alkanes [6,8,18,19]. This behavior stems from low temperature reactions involving hydrocarbon radicals and molecular oxygen [19]. Therefore, a comprehensive detailed DME kinetic model for gas turbine and engine applications should correctly predict these low-temperature autoignition features.

Due to the lack of ignition studies at elevated pressures and low-to-intermediate temperatures noted above, the focus of this work is to further the understanding of DME autoignition behavior under such conditions. Autoignition experiments are conducted for DME/oxidizer mixtures in a rapid compression machine (RCM) over a range of compressed pressures, compressed temperatures, and equivalence ratios. This experimental dataset is then used as a basis for validation and refinement of recently developed kinetic models for DME oxidation, with special emphasis on prediction of autoignition characteristics.

2. Experimental

The RCM system used in the present investigation has been described in detail previously [20,21] and only a brief overview will be given here. The RCM consists of a driver piston, a reactor piston, a hydraulic motion control chamber, and a driving air tank. The driver cylinder has a bore of 12.7 cm and the reactor cylinder bore is 5 cm. The machine is pneumatically driven and hydraulically stopped. The machine allows variations of stroke and clearance height. The reaction chamber is equipped with sensing devices for measuring pressure and temperature, gas inlet/outlet ports for preparing the reactant mixture, and quartz windows for optical access. Additionally, the machine incorporates an optimized creviced piston head design to promote a homogeneous and adiabatic zone at the core of the reaction chamber [20]. Homogeneous reactant mixtures are prepared manometrically inside a mixing tank equipped with a magnetic stirrer.

DME/O₂/N₂ mixtures are studied over the temperature range of 615–735 K, pressure range of 10–20 bar, and equivalence ratio range of 0.43–1.5. Table 1 lists the compositions of gas mixtures tested herein. Note that in Table 1, equivalence ratio (ϕ) is changed by altering the mole fractions of O₂ and N₂ while keeping a constant mole fraction of DME. Here, equivalence ratio is calculated by $\phi = 3 X_{\text{DME}}/X_{\text{O}_2}$, where

Table 1 – Molar composition and stoichiometries of gas mixtures tested

DME	O ₂	N ₂	ϕ	ϕ_{Ω}
1	7	27	0.43	0.47
1	4	30	0.75	0.78
1	2	32	1.50	1.40

X_{DME} and X_{O_2} are the mole fractions of DME and O₂, respectively. In certain studies, especially those dealing with emissions [22], ϕ may not be a good measure of mixture stoichiometry in comparing properties of oxygenated versus non-oxygenated fuels. In these cases, the definition of an “oxygen equivalence ratio,” ϕ_{Ω} [22,23], becomes relevant. For the purposes of the present study, however, the use of ϕ is sufficient as no comparisons to other fuels are performed and the main interest is in examining the temperature and pressure dependence of DME autoignition. For oxygenated hydrocarbon fuels (i.e. those containing H, C, and O) ϕ_{Ω} is defined as the amount of oxygen atoms required to convert all C and H atoms in the fuel/oxidizer mixture to CO₂ and H₂O divided by the amount of oxygen atoms present in the fuel/oxidizer mixture. For the present DME mixtures, $\phi_{\Omega} = 7X_{\text{DME}}/(X_{\text{DME}} + 2X_{\text{O}_2})$ or $\phi_{\Omega} = 7\phi/(6 + \phi)$. The oxygen equivalence ratio is also listed in Table 1. Note that the two definitions vary by no more than 9% over the conditions studied. In this RCM investigation, DME (supplied by Fisher Scientific) is 99.5% pure; O₂ and N₂ gases (supplied by Praxair) are of ultra high purity (99.993% and 99.999%, respectively). For a given mixture composition with known initial temperature, the compressed gas temperature at the end of the compression stroke (top dead center, TDC), T_c , is varied by altering the compression ratio; whereas the desired pressure at TDC is obtained by varying the initial pressure of the reacting mixture for a given compression ratio. The temperature at TDC is determined from measured pressures by the adiabatic core hypothesis according to the relation

$$\int_{T_0}^{T_c} \frac{\gamma}{\gamma - 1} \frac{dT}{T} = \ln\left(\frac{P_c}{P_0}\right)$$

where P_0 is the initial pressure, T_0 is the initial temperature, γ is the temperature-dependent specific heat ratio, and P_c is the measured pressure at TDC.

3. Numerical modeling

Due to heat loss to the combustion chamber walls, compression in an RCM is not truly adiabatic, and the pressure also decreases during the post-compression period. Consequently, a numerical model that accounts for the effect of heat loss is required to correctly simulate the RCM experimental data. For a properly designed creviced piston, such as the one used in the present experiments, isentropic core compression can be assumed and the effect of heat losses can be represented numerically by comparing the computed and measured pressure traces [21]. Compression may also be non-ideal due to small amounts of piston blow-by, but the method described below also accounts for this effect as well. In the present study, non-adiabatic effects are expressed through an adiabatic expansion by prescribing an

Download English Version:

<https://daneshyari.com/en/article/211067>

Download Persian Version:

<https://daneshyari.com/article/211067>

[Daneshyari.com](https://daneshyari.com)