



Burning velocities and jet-stirred reactor oxidation of diethyl carbonate

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Abstract

There is current interest in utilizing oxygenated biofuels such as carbonates in blends with conventional oil-derived liquid fuels. Carbonates, commonly used as electrolyte solvents in Li-ion cells, could ignite after abusive operating conditions. Improving the kinetic modeling of the oxidation of these bio-derived oxygenates requires further investigation under well-controlled conditions. An experimental and detailed chemical kinetic modeling study of diethyl carbonate (DEC) oxidation and combustion was performed. Experiments were carried out in a jet stirred reactor over a wide range of equivalence ratios, temperatures, and pressure. Mole fractions of stable species were measured in the jet stirred reactor at atmospheric pressure. Burning velocities of DEC/air mixtures were determined at elevated temperature over a range of pressures and equivalence ratios. A detailed chemical kinetic modeling was performed using the present experimental results and existing literature data and model. The model represents fairly well the present data. Sensitivity and reaction paths analyses were used to rationalize the results.

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1. Introduction

Whereas search for renewable fuels develops, there is urgent need to provide experimental data and kinetic models applicable to the ignition, oxidation, and combustion of biofuels for fire safety, automotive engines, and gas turbines. Diethyl carbonate (DEC, CAS 105-58-8) is a bio-derived fuel

of much interest because it can be produced from bio-ethanol, itself obtained from agricultural or forestry waste, lignocellulose, sugar beet, sugarcane, or other agricultural crops. Unlike ethanol [1], DEC can be easily mixed with commercial diesel fuel. According to previous studies, adding DEC to diesel fuel has several advantages, among which the reduction of particulate emissions from a diesel engines [2]. This is particularly important when it is desirable to reduce pollutant emissions from legacy fleets of diesel vehicles not equipped with

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particulate traps. Recently, DEC has drawn significant attention in the literature. By testing different oxygenated fuels in engines, it was found that DEC yielded important reduction in particulate emissions [3,4]. Laboratory premixed-flame measurements also indicated a reduction of soot production as well as a reduction of the quantity of PAHs present on soot by adding 20 vol% of DEC to Jet A1 [5]. Nakamura et al. [6] recently presented an experimental and kinetic modeling study of the high-pressure ignition of DEC in a RCM and a shock tube at 30 atm and of DEC oxidation in a jet-stirred reactor (JSR) at 10 atm. Although it is well-known that total pressure can strongly influence oxidation pathways, the former study was limited to high-pressure conditions relevant to internal combustion engines and gas turbines operation. However, the combustion of DEC at atmospheric pressure is also of interest. This is relevant to safety issues associated to abusive operating conditions of Li-ion cells containing carbonates (common electrolyte solvents) that can be released and ignited by accident [7]. However, no previous burning velocity measurement has been presented for DEC/air mixtures. Therefore, in order to further test the kinetic model proposed earlier [6], new experiments must be performed at atmospheric pressure.

The goal of the present study was two-fold: (i) obtain archival experimental data on the oxidation and combustion of DEC over a wide range of equivalence ratios and temperatures, and (ii) use the present experimental data along with available literature data to validate a DEC reaction kinetic mechanism that covers both low- and high-temperature oxidation regimes.

2. Experimental

2.1. The jet-stirred reactor

The experimental setup used here has been described earlier [8,9]. The present experiments were performed at steady state, at a constant pressure of 1 atm, and a constant mean residence time $\tau = 0.07$ s. The volume of the fused silica spherical reactor was 38 cm³. The reactants flowed continuously into the JSR and the temperature of the gases inside the reactor was increased stepwise. Before reaching the injectors, the reactants were diluted with nitrogen (< 100 ppm H₂O, < 50 ppm O₂, < 1000 ppm Ar, < 5 ppm H₂). The fuel-nitrogen mixture flowed through a capillary whereas the oxygen-nitrogen mixture flowed around the capillary, inside the upper reactor extension tube. The two flows mixed in a small volume before entering the four 1 mm tip injectors. A high degree of dilution (0.1 mol% of fuel) was used, reducing temperature gradients in the JSR and heat release. The reactants were high-purity oxygen (99.995% pure) and high-purity anhydrous DEC

(>99% pure, Sigma-Aldrich). The reactants were preheated before injection to minimize temperature gradients inside the reactor. A HPLC pump with an on-line degasser was used to deliver the fuel to an atomizer-vaporizer assembly maintained at 403 K. Good thermal homogeneity along the vertical axis of the reactor (gradients of ca. 1 K/cm) was observed during the experiments by thermocouple measurements (0.1 mm Pt–Pt/Rh-10%, located inside a thin-wall silica tube). The reacting mixtures were sampled by a movable fused silica low-pressure sonic probe, and sent to analyzers via a Teflon heated line maintained at 403 K. The samples were analyzed online by FTIR (10 m path-length, 200 mbar, resolution of 0.5 cm⁻¹) and gas chromatography (GC, Shimadzu QP-2010 SE) and off-line by GC, after collection and storage in 1 L Pyrex bulbs. For GC analyses we used GC equipped with capillary columns (DB-624, CP-Al₂O₃-KCl, and Carboplot-P7), a TCD (thermal conductivity detector), and an FID (flame ionization detector). GC–MS (Varian quadrupole V1200 and Shimadzu QP-2010 SE) operating with electron ionization (70 eV) were used for products identification.

2.2. The combustion chamber

Experiments for determining burning velocities of DEC/air flames were carried out in a pressure-release type dual chamber. It consists of a stainless steel spherical combustion chamber (named IHP) affording a volume of 1 l which is centered in an octagonal high pressure chamber (named CHP) of 10 l. It follows the concept initially introduced by Tse et al. [10] in 2000. To achieve higher pressures, Tse et al. [10] introduced a dual-chamber design in which the wall of the inner chamber is fitted with a series of holes that can be mechanically opened and closed to allow the union and separation of the gases. In 2005, Qin and Ju [11] then modified the dual chamber design of [10] and introduced magnetically controlled gates to automatically relieve the pressure to the outer chamber. To enable measurements for liquid fuels flames, Kelley et al. [12] adopted electrical heaters and obtained uniform heating of the vessel up to 380 K and Santner et al. [13] adopted an external heating oven to perform experiments for fuels with boiling temperature up to 500 K.

The current combustion chamber [14] is equipped with 6 evacuation valves which are distributed around in a symmetrical configuration. The external chamber is filled with inert gas while the spherical combustion chamber is filled at the same pressure with the test mixture. The evacuation valves are mechanically adjusted via springs calibrated to open at a fixed overpressure. When the overpressure between the two chambers reaches 0.025 MPa, the valves open, resulting in an expanding flame that propagates in the inner

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