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A comprehensively validated compact mechanism for dimethyl ether oxidation: an experimental and computational study



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ABSTRACT

Dimethyl ether (DME) is regarded as one of the most promising alternatives to fossil fuels used in compression ignition engines. In order to critically evaluate its overall combustion behaviour via numerical simulations, an accurate as well as compact kinetic mechanism to describe its oxidation is most essential. In the present study, a short kinetic mechanism consisting of 23 species and 89 reactions is proposed to describe the oxidation of DME. This is based on the detailed San Diego mechanism. The short mechanism accurately reproduces the available experimental data for ignition delays, laminar flame speeds, and species profiles in flow reactors as well as jet-stirred reactors. To assess the validity of this reaction mechanism in non-premixed systems, extinction strain rates of DME-air mixtures, which are not available in the literature, are measured in a counter-flow diffusion flame burner as a part of the present work. The 23 species reaction mechanism is also able to predict the experimental data for extinction within the uncertainty limits. This mechanism is further reduced by introducing quasi-steady state assumptions for six intermediate species to finally obtain a 14-step global kinetic scheme. A code is developed in MATLAB to obtain these 14 global steps and their corresponding rate expressions in terms of the individual reaction rates. The 14-step mechanism performs as good as the 23 species mechanism for all the experimental data sets tested for.

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detailed mechanisms have been proposed for DME oxidation. Da-

1. Introduction

Emissions from automobiles, especially that from compression ignition engines, significantly contribute to environmental pollution. An attractive way to tackle this problem is to use alternative fuels. Dimethyl ether (DME) is one such fuel, which can replace fossil diesel for use in compression ignition engines [1]. The high cetane number (55–60) [2] of DME and ease of its handling (remains a liquid when pressurized above 0.5 MPa) makes it particularly attractive for use in such applications [3]. The fast evaporation rate of DME leads to better mixing with air within the engine and its inherent oxygen content helps achieve smokeless combustion through reduced formation and high oxidation rates of particulates. In fact, diesel-DME blends have been shown to result in reduced soot precursors than neat diesel [2,4–6].

Significant amount of research, both based on experiments and modeling, has been undertaken on DME kinetics [7–12]. Several

gaut et al. [7,8] proposed a detailed reaction mechanism with 331 reactions involving 55 species to describe the low and high temperature oxidation of DME in a jet-stirred reactor (JSR) (550-1275 K, 1–10 atm) as well as the ignition of DME in shock tubes (650-1600 K, 3.5-40 bar). Curran et al. [9] developed a detailed kinetic model for DME oxidation and demonstrated its validity in JSR and shock tube configurations over a wide range of conditions (650-1300 K, 0.2-2.5, 1-40 atm). This model incorporated 336 reactions among 78 species. Some modifications were introduced to this kinetic scheme by Curran et al. [10] to additionally describe the oxidation of DME in a variable pressure flow reactor. Fischer et al. [11] further modified the mechanism proposed by Curran et al. [10] to extend its validity to include the pyrolysis of DME at high temperatures. Zhao et al. [12] developed a comprehensive model for DME pyrolysis and oxidation in a hierarchial manner. This model, consisting of 290 reactions among 55 species, showed a good agreement against flow reactor, JSR data, shock tube ignition delays, and laminar flame speed measurements.

In a recent study, Burke et al. [13] proposed a detailed kinetic mechanism for DME oxidation by incorporating accurate rate constant measurements and calculations for the reactions of DME.

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The mechanism was also the first to employ a pressure-dependent treatment to the low temperature reactions of DME. It was validated using data available in the literature including, species profiles in flow reactor and JSR, shock tube ignition delay times, and flame speeds. Prince and Williams [14] came up with a 14-step DME sub-mechanism, to be combined with the San Diego mechanism [15], which was successfully tested against the aforementioned data sets as well. Dames et al. [16] developed a binary fuel kinetic model for DME and propane with focus on engine-relevant conditions (10–50 atm and 550–2000 K). The model (120 species and 711 reactions) was further validated against rapid compression machine (RCM) data for DME-propane mixtures.

Although detailed mechanisms provide accurate predictive capabilities, the computational time and complexities involved are large, which essentially constrains their use in multi-dimensional computations. This has propelled the development of compact reaction mechanisms for DME oxidation [17-22]. Beeckmann et al. [17] proposed a reduced reaction mechanism, specifically to capture the autoignition of DME. Pan et al. [18] (29 species and 66 reactions), Yamada et al. [19] (23 species and 23 reactions), Kim et al. [20] (28 species and 45 reactions), and Chin et al. [21] (28 species) came up with skeletal/reduced models particularly applicable to engine combustion. Chang et al. [22] developed a reduced chemical mechanism for DME using a decoupling methodology, wherein the rate parameters in the DME sub-mechanism were optimized to match the experimental data (shock tubes, flow reactors, JSR data, and flame speeds). Nonetheless, the size of this mechanism (42 species and 171 reactions) remains comparable to some of the detailed mechanisms discussed above.

Despite the availability of several short reaction mechanisms for DME oxidation, their range of validity is limited to specific configurations. However, in many combustion systems, the precise manner in which the combustion process advances is not known apriori. For instance, there may exist regions within a system where ignition and premixed flame propagation are dominant, while in others, diffusion governs the combustion process. Therefore, in order to be integrated with simulations of combustion systems in general, the short mechanism for DME oxidation should be applicable to a wide range of combustion configurations.

Thus, the objectives of this work are two-fold: (i) develop a short mechanism for DME oxidation that is as compact as possible, still containing the essential kinetics and (ii) ensure that the proposed mechanism is validated comprehensively to establish its ability to accurately predict a wide range of configurations of practical relevance to combustion. In view of the second objective, while significant data is available in literature for validation of DME kinetics in premixed environment, for instance, Refs. [7,8,10,11,13], there is a lack of experimental data in non-premixed systems. Thus, as a part of this work, extinction strain rates of DME-air mixtures have been obtained in a counter-flow non-premixed flame, thus expanding on the available database for kinetic model validation.

This work is organized as follows. First, the experimental methodology to measure extinction strain rates in a 1D laminar non-premixed counter-flow burner is presented (Section 2). Thereafter, following a similar approach to the development of a short kinetic model for methanol oxidation by Tarrazo et al. [23], a compact mechanism is developed for DME oxidation (discussed in Section 3). An extensive validation of the compact reaction scheme against available experimental data for constant volume and constant pressure homogeneous reactors, unstretched laminar premixed flames, and well-stirred reactor as well as the measured extinction strain rates is presented in Section 4. To further simplify this mechanism and subsequently reduce the computational cost when using in combustion simulations, quasi-steady state assumption has been invoked for a few intermediate species. A reduced

mechanism is thus arrived at for DME oxidation. Computations are performed to validate the results from this reduced mechanism against all experimental data sets (discussed in Section 5). Following this, the article is concluded by summarizing the contributions and highlighting the principal findings.

2. Counter-flow diffusion flame extinction experiments

Significant data is available in literature for validating DME kinetic models in a premixed environment, for instance, Refs. [7,8,10,11,13]. Along with configurations in a premixed system (such as shock tubes, flow reactors, and flame speeds), extinction strain rates in non-premixed flames are particularly important for validating a reaction scheme because it verifies the interplay between the time scales of kinetics and diffusion processes, which compete with each other during extinction. Wang et al. [24] obtained extinction strain rates of DME-oxygen mixtures at atmospheric pressure and elevated unburnt mixture temperature in a counter-flow diffusion flame. Since most of the practical combustion systems use air as the oxidizer, as a part of the present work, experiments have been performed in a canonical 1D counter-flow configuration to obtain the extinction strain rates of DME-air mixtures in nonpremixed flames. In the present work, strain rates at extinction are experimentally measured as a function of the mass fraction of fuel in the fuel stream (Y_{E1}) . This experimental data set acts as a validation target for the proposed short mechanism.

2.1. Experimental apparatus

The counter-flow burner setup used in the present work is manufactured at UCSD and an exactly similar setup has been previously used by the UCSD group to measure the extinction and autoignition characteristics of several fuels [25,26].

A schematic of the counter-flow burner setup used in the present study is shown in Fig. 1. It consists of fuel (bottom) and oxidizer (top) ducts, kept co-axially opposing each other. The fuel duct ($d_f = 25.4$ mm) is surrounded by two concentric annular ducts. Nitrogen is supplied through the inner annular gap in order to minimize the effect of ambient interference. The outermost annular duct is connected to an exhaust system, which facilitates the suction of the hot product gases. The outer walls of this duct are provided with water spray nozzles (type BETE PJ15) to cool the hot product gases and thereby prevent their autoignition in the exhaust duct. Water is supplied to the spray nozzles through a mini centrifugal pump (TULLU AC-30). The oxidizer duct ($d_{ox} = 25.4$ mm) is surrounded by a concentric duct through which nitrogen is supplied, similar to that used in the fuel duct.

Plug-flow boundary condition is ensured by placing multiple stainless steel wire screens (200 meshes/inch) near the exits of both fuel and oxidizer ducts. The flow rates of DME, air and nitrogen are controlled using rotameters (with an uncertainty 2% of full scale reading). The fuel and nitrogen are mixed in a cylindrical mixing chamber of diameter 50 mm and length 200 mm. A series of fine stainless steel meshes are arranged inside the mixing chamber in order to ensure a homogeneous mixture.

2.2. Experimental procedure

Before starting the experiment, the water cooling system is turned on. First, a stable flame is established by controlling the flow rate of DME through the fuel duct and by introducing a small pilot flame for ignition. The exhaust system is switched on immediately after the ignition to vent out hot products gases. Once the flame is stabilized, air is allowed to enter through the oxidizer duct to establish a flat flame as shown in Fig. 2(a). The curtain flow of nitrogen in both the ducts is adjusted using separate rotameters. Download English Version:

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