Fuel 160 (2015) 165–177

Contents lists available at ScienceDirect

Fuel

journal homepage: www.elsevier.com/locate/fuel

Development and validation of a reduced chemical kinetic model for dimethyl ether combustion

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HIGHLIGHTS

- A reduced DME mechanism is proposed for ignition delay and combustion predictions.
- The reduced mechanism was validated against experimental ignition delay times.
- The reduced mechanism was validated against the parent mechanism.
- The reduced mechanism was validated against engine and emissions data.

ARTICLE INFO

Article history:
Received 13 May 2015
Received in revised form 14 July 2015
Accepted 20 July 2015
Available online 1 August 2015

Keywords:
Dimethyl ether
Reduced reaction mechanism
CFD
Combustion

ABSTRACT

A new, reduced reaction mechanism for DME combustion in internal combustion engines is proposed. The new mechanism is based on a detailed DME mechanism suitable for low to high temperature ranges. The reduced model consists of 29 species and 66 reactions and contains a detailed H_2/CO mechanism and reduced C1–C2 chemistry. The reduced mechanism inherits the major reaction pathways of the detailed mechanism, which ensures its predictive capability when coupled into CFD simulations. The performance of the reduced mechanism was compared to simulation results of the detailed mechanism, ignition delay times from a shock tube and a rapid compression machine, and DME engine combustion data. Overall, the reduced mechanism shows a good balance between accuracy and computational efficiency necessary for use in combustion system design applications.

1. Introduction

Increasingly stringent pollutant regulations and increasing energy demand have driven the need for development of high-efficiency combustion technologies and alternative fuels for cleaner, more efficient, environmentally sustainable combustion. Recently, highly premixed, low temperature combustion (LTC) technologies including homogeneous charge compression ignition (HCCI), premixed charge compression ignition (PCCI) and reactivity controlled compression ignition (RCCI) have attracted great attention, because they can provide higher thermal efficiency, lower nitrogen oxide (NOx) and soot emissions than conventional diesel engines [1]. The combustion event, performance, and emissions characteristics of these novel combustion technologies are typically controlled by the fuels auto-ignition characteristics, highlighting the importance of the fuel's chemical properties [2]. Thus, accurate chemical kinetic mechanisms are of great importance for simulation of advanced engine combustion concepts [3].

Dimethyl ether (DME) is a promising alternative fuel for compression ignition engines since it can provide low PM or soot emissions and be synthesized from emerging renewable energy sources, such as biomass and existing fossil fuel sources [4]. Furthermore, DME offers favorable combustion characteristics including easily auto-ignited due to a high cetane number and soot-free combustion due to the easy vaporization and no carbon–carbon bond [5]. Accordingly, many DME spray [6–12] and engine investigations [5,13–19] have been performed in recent years. Suh and Lee [6] investigated the macroscopic and atomization characteristics of DME and diesel fuel using a common-rail injection system in a compression ignition engine. They found that the DME spray is wider, shorter, and evaporates more rapidly than diesel spray under identical injection conditions. Recently, Konno et al. [20] studied DME spray characteristics at injection pressures up to 140 MPa in a constant volume vessel under engine-like temperature/pressure conditions. Their results confirmed the results of Suh and Lee [6], showing that the evaporation of DME is much

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http://dx.doi.org/10.1016/j.fuel.2015.07.066
0016-2361/

Nomenclature

DME	dimethyl ether	IC engine	internal combustion engine
CFD	computational fluid dynamic	NTC	negative temperature coefficient
LTC	low temperature combustion	RCM	rapid compression machine
HCCI	homogeneous charge compression ignition	ST	shock tube
PCCI	premixed charge compression ignition	IMEP	indicated mean effective pressure
RCCI	reactivity controlled compression ignition	SOI	start of injection
NOx	nitrogen oxide	ATDC	after top dead center
HC	hydrocarbon	TDC	top dead center
CO	carbon monoxide	ERC	Engine Research Center
JSR	jet stirred reactors		

faster than that of diesel fuel, resulting in a more evenly distributed spray. Youn et al. [21] compared the combustion and emissions characteristics of DME to conventional diesel fuels in a four-cylinder compression ignition engine under various operating conditions. They concluded that, when operated at the same engine load, the DME fueled engine has a higher peak combustion pressure and shorter ignition delay than the diesel fueled engine. They also found that the DME fueled engine provides lower soot, hydrocarbon (HC) and carbon monoxide (CO) emissions and slightly higher NOx emission than the diesel fueled engine. Recently, Park et al. [18] reviewed the physical and chemical properties, spray atomization characteristics, combustion, and exhaust emission characteristics of DME and concluded that DME is a promising alternative fuel for internal combustion engines and it can be used in place of conventional diesel fuel in compression ignition engines.

Beyond spray and engine studies, DME has been the subject of numerous fundamental experimental studies, including ignition delay times [22–30], premixed laminar flames [31–36], pyrolysis chemistry and oxidation chemistry [36–39]. These experimental studies are of great value for validation and construction of chemical kinetic mechanisms describing DME oxidation. Dagaut et al. [39] proposed a semi-detailed kinetic model of DME containing 43 species and 286 reactions. It was able to reproduce species

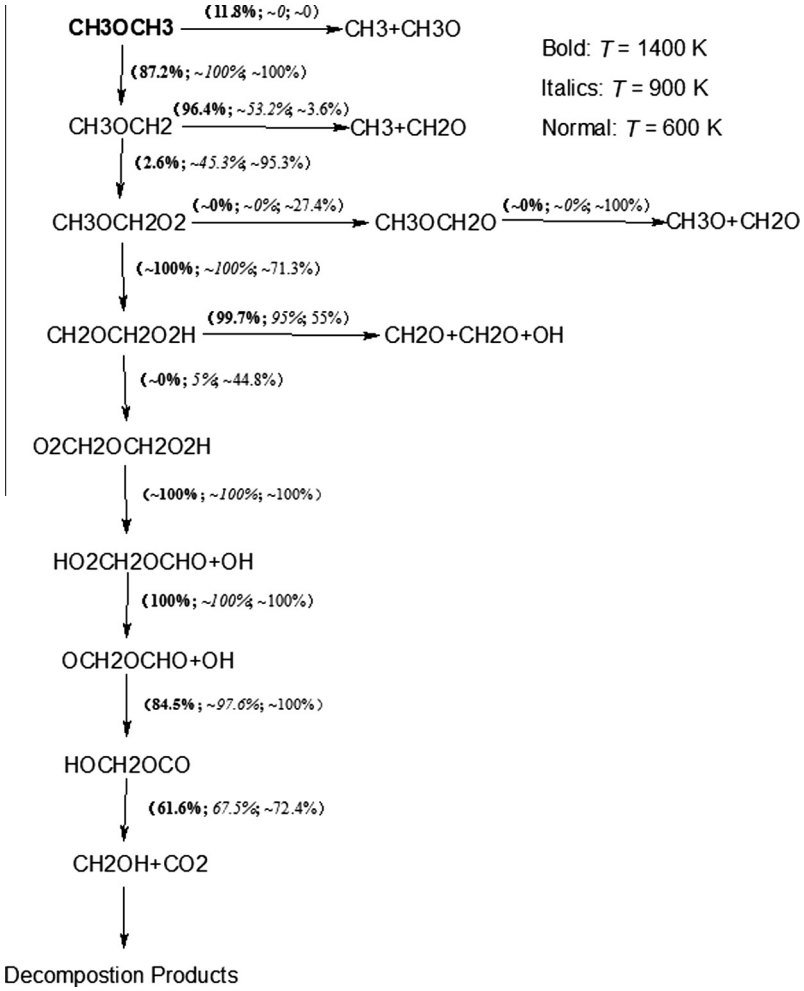

Fig. 1. Reaction pathway diagram for stoichiometric DME/air mixture at $p = 50$ atm using NUIG Mech_56.54.