



# A skeletal mechanism for multi-component fuel combustion simulations



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## HIGHLIGHTS

- Skeletal kinetics was constructed for multi-component fuels with 132 species.
- Derived mechanism can treat diesel, biodiesel, ethanol and DMC oxidation reactions.
- CO, NO<sub>x</sub> and soot formation mechanisms are embedded.
- It was well validated against detailed reaction mechanism and experimental results.

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## ABSTRACT

The present study aims to develop a skeletal mechanism for multi-component fuel oxidation of diesel, biodiesel blended with short chain oxygenated fuels of ethanol and DMC. Starting from a detailed reaction mechanism, a reduced chemical kinetics which could treat both ethanol and DMC oxidation reactions was first developed using directed relation graph with error propagation and sensitivity analysis (DRGEPSA) method, and it was then combined with a tri-component biodiesel reaction mechanism developed in our previous study with CO, NO<sub>x</sub> and soot emission sub-models embedded. The final mechanism comprises 132 species and 617 elementary reactions. Extensive validations were performed for the developed skeletal mechanism through ignition delay testing and 3-D engine simulations. Validation results discerned that for ethanol, DMC and diesel fuels, predicted ignition delay time agreed very well with the detailed reaction mechanism or experimental results over a large range of initial pressure, temperature and equivalent ratio conditions with the maximum deviation below 25%, whereas for biodiesel, the largest discrepancy was 53%. 3-D engine combustion simulations also demonstrated that the ignition delay, cylinder pressure and heat release rate of diesel, biodiesel and their blend fuels with DMC could be very well reproduced by the present mechanism with reliable accuracies under various engine operating conditions.

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## 1. Introduction

In recent years, the use of oxygenated fuels to modify fuel compositions in the form of additives has become one of the major research activities in the area of combustion, aiming at reducing the polycyclic aromatic hydrocarbons (PAHs) and particulate matter (PM) emissions from diesel engines. The idea of using oxygenated fuels was first introduced as an octane replacement for lead in gasoline engine, and was later recognized for its ability to reduce carbon monoxide (CO) and soot emissions [1]. Oxygenated fuels are nothing but those chemical compounds which contain oxygen atoms in their chemical structures, usually in the form of alcohols such as methanol, ethanol, isopropyl alcohol, and n-butanol or

ethers such as dimethyl ether (DME), methyl tert-butyl ether (MTBE), tertiary amyl methyl ether (TAME), as well as other compounds such as dimethyl and diethyl carbonates.

Since earlier times, numerous studies [1–9] have been devoted to investigate the impacts of oxygenated fuels on the combustion chemistry of various petroleum fuels, as well as their influences on the performance and emission characteristics of diesel engines. For example, Chen et al. [2] investigated the effects of different oxygenated fuels (methanol, dimethoxymethane, dimethylcarbonate) on laminar premixed n-heptane flames using synchrotron photoionization and molecular-beam mass spectrometry techniques. Together with numerical modeling, mole fraction profiles of major and intermediate species were compared and analyzed. It was discerned that the mole fractions of most C<sub>1</sub>–C<sub>5</sub> hydrocarbon intermediates which were normalized by inlet carbon flux were reduced by 10–30% when oxygenated fuels were added.

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Meanwhile, the benzene ( $C_6H_6$ ) mole fraction was shown to reduce apparently (up to 40%), and its extent of reduction showed little effect among different oxygenated fuels investigated. A similar conclusion was also drawn by Inal and Senkan [1] who compared the effects of three oxygenate additives (methanol, ethanol and MTBE) on the suppression of polycyclic aromatic hydrocarbons and soot formations in laminar, premixed fuel rich flames of n-heptane. It was determined that the extent of reduction by each oxygenate additive was similar and the effect of fuel structure was not very significant. Another computer simulation work was performed by Böhm and Braun-Unkloff [3] using SENKIN code to investigate the impacts of oxygenated compounds and isobutene addition on the PAHs and soot formation from benzene–argon mixtures in shock tubes. It was identified that depending on the amount of blending compounds MTBE, isobutene, methanol and ethanol added to the benzene–argon mixture, the soot-suppressing and soot-promoting effects might vary from each other. It was further discerned that the product of the mole fractions of acetylene and PAHs reasonably reflected the change of soot-promoting into soot-suppressing effects of oxygenated blending compounds and isobutene. For diesel engine applications, Wang et al. [4] experimentally explored the possibility of significantly reducing PM emissions from a diesel engine through blend fuel design. A set of design principles were proposed which require high oxygen content, high cetane number, low sulfur, low aromatics and suitable viscosity. Based on the proposed principles, various blend fuels with different concentrations of biodiesel, ethanol, dimethyl carbonate (DMC) and diesel were prepared and compared. It was found that the oxygenated fuel formulated using 50% biodiesel, 15% DMC and 35% diesel appeared to be the best design which could meet the Euro IV emission standards for heavy-duty diesel engines without the use of any after-treatment devices. Xu et al. [5] analyzed the mechanism of the inhibition effect of methanol on the ignition of long-chain alkane under low and intermediate temperature conditions. A skeletal kinematic model consisting of 30 species participating in 38 elementary reactions was created and validated by the ignition delay predictions of n-heptane, methanol and their blend fuels against the experimental results under various equivalence ratios, initial temperatures and pressures. Additional 3D HCCI engine simulations also verified that the ignition, in-cylinder temperature and the major species had satisfactory predictions. It was claimed that the inhibition effect was the result of methanol transforming the active radical OH into inactive  $H_2O_2$  and the latter accumulated to a large amount under lower temperatures, decreasing the activity of the system and delaying the ignition.

Besides the above studies, there are also some researches [10–16] focusing on the numerical modeling on the combustion process of oxygenated fuels. As one of the earlier works, Fisher et al. [10] developed detailed reaction mechanisms for the combustion of methyl butanoate and methyl formate following the rules developed for hydrocarbon fuels. Derived mechanisms were validated against limited combustion data under low temperature and sub-atmospheric conditions. Marinov [11] constructed a detailed chemical kinetics for ethanol combustion simulations, and its predictions for laminar flame speed, ignition delay and species concentration profiles were validated against various experimental results. Glaude et al. [12] proposed a chemical kinetic model for DMC, and it was employed to better understand its combustion behaviors in an opposed flow diffusion flame. The predicted species profiles agreed well with the experimentally measured values. It was determined that many of the oxygen atoms in dimethyl carbonate transformed directly into carbon dioxide, weakened its effectiveness for soot suppression. Westbrook et al. [13] worked on a detailed chemical reaction mechanism which was used to describe the combustion process of a group of small alkyl ester

fuels, consisting of methyl formate, methyl acetate, ethyl formate, and ethyl acetate. The resulting mechanism was validated by comparing the predicted mole fractions of intermediate species against those of experimental results for fuel rich, low pressure and premixed laminar flames. For low carbon oxygenated fuels, Tran et al. [17] reviewed the progress made on the development of detailed chemical kinetics. They started by identifying the major species present in the oxygenated fuels obtained from biomass, and summarized the major reaction mechanisms that were proposed in the literature. Further analysis on the specific classes of reactions considered in detailed kinetic models for the combustion of acyclic and cyclic molecules were presented and compared. It was concluded that the mechanisms for the oxidation of saturated cyclic ethers were close to that of cyclic alkanes, however, the reactions for unsaturated cyclic ethers remained complex and uncertain. In addition to the above efforts made for short chain oxygenated fuels, some recent studies [18–21] were carried out to develop detailed or skeletal chemical kinetics for long chain oxygenated biodiesel. However, although many kinetic models have been developed for some individual oxygenated fuels or their surrogate species, the studies focusing on the development of multi-component fuel reaction mechanisms are rather rare, especially for the blend fuels of diesel, biodiesel with short chain oxygenated fuels.

The objective of this study is to bridge the gap to develop a skeletal multi-component kinetic model for the oxidation of automobile fuels of diesel, biodiesel blended with short chain oxygenated fuels of ethanol and DMC. Starting from a detailed reaction mechanism [12] which considers both the ethanol and DMC reaction pathways, a skeletal reaction mechanism was built using directed relation graph with error propagation and sensitivity analysis (DRGEPSA) method [22], and was further combined with a tri-component skeletal mechanism of biodiesel (Biodiesel-An mechanism) developed by An et al. [18]. Improvements were made to the constructed multi-component fuel chemistry by performing constant volume SENKIN analysis and reaction rate optimizations for selected reactions. Derived chemical reaction model was validated by comparing ignition delay predictions against those of detailed reaction mechanisms or against shock tube experimental data available in the literature. To further examine its applicability in diesel engine simulations, 3D numerical simulations were conducted using coupled KIVA4-CHEMKIN code, and predicted cylinder pressure and heat release rate curves were compared against the experimental results. Following similar approaches that were used in our earlier studies [23,24], the chemical and thermo-physical properties of DMC were predicted.

## 2. Methodology

### 2.1. Experimental approach

With the objective of analyzing the applicability of the proposed multi-component surrogate mechanism in diesel engine and validating its prediction accuracies on in-cylinder pressure and heat release rate, a light duty, four-cylinder, four-stroke, turbo-charged, direct injection diesel engine with a compression ratio of 18.5 was employed in this investigation. Fig. 1 shows a schematic diagram of the engine setup and Table 1 lists the major specifications of the engine. The test engine was directly loaded with an AVL DP 160 dynamometer which could provide a maximum braking power of 160 KW and a maximum torque of 400 Nm with an accuracy of  $\pm 0.3\%$ . Various sensors and performance indicating system were installed and connected to the test engine. Particularly, the in-cylinder pressure was measured using an AVL GH13P water-cooled pressure transducer mounted on the first cylinder

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