



# Development of a skeletal mechanism for biodiesel blend surrogates with varying fatty acid methyl esters proportion



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## HIGHLIGHTS

- A new biodiesel skeletal mechanism is developed in this work.
- The skeletal mechanism can be used for biodiesel with varying FAMES proportion.
- Three tests were performed and the calculation results were very well.

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## ABSTRACT

A skeletal four-component biodiesel combustion mechanism comprising methyl decanoate, methyl-5-decenoate, *n*-decane and methyl linoleate is proposed in the present study. The motivation of this work is to develop a mechanism for accurate modeling on the effect of varying fatty acid methyl ester proportion on biodiesel ignition and combustion. The skeletal mechanism was generated by coupling an existed methyl decanoate, methyl-5-decenoate, *n*-decane skeletal mechanism with a new developed skeletal methyl linoleate mechanism, which was reduced from a penta-component detailed mechanism consisting of 5025 species and 20,163 reactions. The employed reduction strategies are directed relation graph error propagation and sensitivity analysis (DRGEP-SA), isomer lumping, computational singular perturbation and reaction rate adjustment. The skeletal methyl linoleate mechanism consists of 92 species and 249 reactions, and the coupled biodiesel blend surrogates mechanism consists of 106 species and 263 reactions. In order to validate the feasibility of the new developed skeletal mechanism, zero-dimension ignition delay testing, reflected shock tube experiment validation and 3-dimensional engine testing about cylinder pressures, heat release rates and NO<sub>x</sub> emission trends were conducted at different conditions. And the new developed skeletal mechanism was compared with a biodiesel surrogates skeletal mechanism without double-bond species in the 3-dimensional engine testing. The results indicate that the new developed skeletal mechanism is suitable to predict ignition behavior, combustion characteristics, NO<sub>x</sub> emission trends of biodiesel with varying fatty acid methyl ester, and it is more accurate than a biodiesel surrogates skeletal mechanism without double-bond species in the 3-dimensional engine testing.

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## 1. Introduction

With the depletion of fossil fuels, developing some suitable alternative fuels is imminent. Biodiesel is regarded as a promising candidate to substitute fossil diesel due to their similar physico-chemical characteristics, which allows biodiesel to be used in diesel engine with minimal or no modifications [1]. Biodiesel is a fuel made up of multi-component mixture of long carbon chain fatty

acids methyl esters (FAMES), derived from animal fats or vegetable oils by transesterification process [2]. Actually, the biodiesel fuels are mainly synthesized from vegetables such as peanut and rapeseed, since vegetable oils are ready available with lower sulfur and aromatic content compared to animal fat [2,3]. Moreover, the use of biodiesel or its blends can reduce the emissions of unburned hydrocarbon (HC), carbon monoxide (CO) and particulate matter (PM), but a slight increase in the nitrogen oxides (NO<sub>x</sub>) emissions [4,5]. However, fuel injection strategy adjustment, multi way catalytic converter post-processing and other engine emission control methods can be employed to reduce the NO<sub>x</sub> emissions [6,7].

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The components of different biodiesels are different. However, most of researches indicated that typical biodiesels mainly contain five components, i.e., methyl palmitate (MP,  $C_{17}H_{34}O_2$ ) and methyl stearate (MS,  $C_{19}H_{38}O_2$ ) as saturated ME, as well as methyl oleate (MO,  $C_{19}H_{36}O_2$ ), methyl linoleate (ML,  $C_{19}H_{34}O_2$ ) and methyl linolenate ( $C_{17}H_{32}O_2$ ) as the unsaturated ME components [1,8,9]. The concentrations of other components are very low and have little effect on the combustion process [2,10]. So, to capture the main combustion characteristics of biodiesel, meanwhile, to save computational time, it is widely recognized to choose some of the major components as surrogate to represent the biodiesel. As a potential substitute to fossil diesel, numerous studies have been performed to explore the applicability of biodiesel in diesel engine, including biodiesel mechanism development [8,11–16], injection strategy optimization [17,18], combustion and emission characteristics analysis [19–21]. Westbrook et al. developed some very important detailed chemical kinetic mechanisms for biodiesel surrogates and different biodiesel blend fuels, for instance, a detailed mechanism for methyl decanoate (MD) [11] has been developed by using systemic rules for *n*-heptane and iso-octane [22,23]. The mechanism is capable of predicting biodiesel or extending to a longer alkane chain. Then detailed mechanisms for methyl-5-decanoate (MD5D) and methyl-9-decanoate (MD9D) [12] were developed based on the detailed mechanism for MD. And a multi-component mechanism including MD, MD9D and *n*-heptane was developed to represent the detailed oxidation mechanism of rapeseed oil. After these, Westbrook et al. had established detailed mechanisms of MS, MO and other major components of biodiesel fuels [8,13]. The development of these detailed mechanisms made a significant contribution to biodiesel research. However, these detailed mechanisms are too big to use in engine simulation, so mechanism reduction methodologies and some feasible skeletal mechanisms were developed. For example, Lu and Law [24] developed a systematic method of directed relation graph (DRG), the method was firstly performed for a detailed ethylene oxidation mechanism reduction, and then validated by calculating laminar flame speeds and non-premixed counterflow ignition. Based on it, some derivative products were proposed such as directed relation graph aided sensitivity analysis (DRGASA) [25], directed relation graph with error propagation (DRGEP) [26], directed relation graph with error propagation and sensitivity analysis (DRGEP-SA) [27]. DRGEP-SA was developed by integrating two previously developed methods DRGASA and DRGEP, and it can reduce many species and reactions with a specified precision requirement of ignition delay time. Other reduction methods such as, sensitivity analysis (SA) [27] can be used for analyzing the effect of “limbo” species on global reaction and then consider to remove some of them, “limbo” species and its details came from Ref. [27]; peak concentration analysis [28] can be used for finding out unimportant species and removing them from mechanism one by one; computational singular perturbation (CSP) [29] is an automatic procedure for the simplification of chemical kinetic mechanisms by eliminating unimportant reactions based on a specified error tolerance; chemical isomer lumping [30] is used to reduce isomer groups. These methods established the cornerstone of mechanism reduction. Luo et al. [14] developed a tri-component (MD, MD9D and *n*-heptane) skeletal mechanism comprising 115 species and 460 reactions, then validated ignition delay times against detailed mechanism, experimental data in specified reactors, and extended validations for premixed and non-premixed flames besides 3-D constant volume combustion chamber validation under CI (compression ignition) engine conditions. Similarly, An et al. [15] developed a MD, MD9D and *n*-heptane skeletal mechanism from an updated LLNL detailed biodiesel oxidation mechanism which consists of 3299 species and 10,806 reactions, then validated their skeletal

mechanism by comparing ignition delay predictions with shock tube experimental data of *n*-heptane and the ignition delay predictions by detailed mechanism in a homogeneous system, and further validated by engine experimental data for cylinder pressure and heat release rate. The final mechanism consists of 112 species and 498 reactions and could be combined with other reduced mechanisms to generate a specified mechanisms of new fuel [16]. Chang et al. developed another tri-component (MD, MD5D and *n*-decane) skeletal mechanism [31] by a decoupling methodology described in their previous work [32]. These skeletal mechanisms were generated by subjecting to a specified range of temperatures, pressures and equivalence ratios, and validated ignition delay time predictions against reflected shock tube experimental data of MD and MD5D determined by Wang et al. [33], species concentrations against experiments in a jet-stirred reactor and engine experimental data for cylinder pressure and heat release rate, the results tended to have a good fitness with original mechanism and experiments.

These skeletal mechanisms have two common features, the first one is reaction rate adjustment as a final step of mechanism reduction. The reaction rate adjustment is performed by adjusting three rate coefficients: pre-exponential factor **A**, temperature exponent **b** or activation energy **E**, just as mentioned in Ref. [28,34]. Actually, some studies prefer to only adjust pre-exponential factor **A** [1,15,16]. Because it is independent of any react conditions, and it would not affect the start of reaction, unlike the activation energy **E**. However, there is some dispute on reaction rate adjustment. Some scholars suggested that these coefficients should not be modified, because the characteristics of reaction would be changed, if its reaction rate coefficients had been modified. But this is a unique situation just for skeletal mechanism. Skeletal mechanism is necessary for engine simulation and the reaction rate adjustment is necessary for skeletal mechanism. Because some slight variation in ignition process is unavoidable by the removal of some species and reaction pathways, in order to minimize this variation and improve the ignition time predictions without changing the number of remained species and reactions, it is necessary to compensate these removed pathways by adjusting reaction rate. The second one is choosing MD, MD5D/MD9D to represent the saturated FAMES and unsaturated FAMES in biodiesel respectively, and *n*-decane/*n*-heptane was chosen to match energy content and C/H/O ratio. However, MD5D or MD9D is a single double-bond methyl ester and the content of two double-bond unsaturated FAMES are not low in biodiesel and should be considered, for example, the content of methyl linoleate ( $C_{19}H_{34}O_2$ ) in soy biodiesel is about 50–60% [13]. Therefore, these reduced mechanisms can't be used for investigating the effect of double-bond content on overall combustion and emission. So, the objective of this work is to develop a suitable skeletal mechanism which can be used for simulating the combustion and emission formation of biodiesel with varying fatty acid methyl ester proportion by using ML ( $C_{19}H_{34}O_2$ ) to represent two double-bond saturated FAMES.

## 2. Methodology

### 2.1. Mechanism reduction strategies

In the present study, methods of DRGEP-SA, peak concentration analysis, isomer lumping, CSP and reaction rate adjustment had been employed to generate a reduced ML mechanism from an penta-component (MP, MS, MO, ML and methyl linolenate) detailed biodiesel mechanism which was developed for the five major components of soy biodiesel and rapeseed biodiesel fuels [13]. Then the reduced ML mechanism would be coupled with a reduced tri-component mechanisms (MD, MD5D, *n*-decane mechanism from the research of Chang et al. [31]). Finally, the new

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