Applied Energy xxx (2014) xxx–xxx

Contents lists available at ScienceDirect

Applied Energy

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

A numerical modeling on the emission characteristics of a diesel engine fueled by diesel and biodiesel blend fuels

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HIGHLIGHTS

- Impacts of biodiesel blend ratio were numerically studied.
- KH–RT breakup model was implemented to increase the accuracy of KIVA–CHEMKIN code.
- A skeletal mechanism was integrated into KIVA for diesel and biodiesel simulation.
- The biodiesel CO emission significantly increased at lower engine loads.
- The CO oxidation window is narrower with the increase of biodiesel blend ratio.

ARTICLE INFO

Article history:
Received 13 October 2013
Received in revised form 12 December 2013
Accepted 2 January 2014
Available online xxxx

Keywords:
Biodiesel
KIVA
Blend ratio

ABSTRACT

A numerical modeling study was performed to investigate the impacts of biodiesel blend ratio on the emission formation processes of a diesel engine. Simulations were conducted using 3-D CFD simulation software KIVA4 coupled with CHEMKIN II. The integrated chemical kinetics with 69 species and 204 reactions comprises the significant reaction pathways of methyl decanoate ($C_{11}H_{22}O_2$), methyl-9-decenoate ($C_{11}H_{20}O_2$) and n-heptane (C_7H_{16}), which are capable of emulating different biodiesel blend ratios. The nitrogen monoxide (NO) and carbon monoxide (CO) formation mechanisms were also embedded. To better represent the biodiesel fuel properties, detailed chemical and thermo-physical properties of biodiesel were calculated and integrated into the KIVA4 fuel library. The simulated cases were validated against the experimental results by comparing the in-cylinder pressure and heat release curves for B100, B50, and pure diesel fuels at 2400 rpm under 10% load, 50% load and 100% load, respectively. Good agreements with a maximum of 5% deviation on the peak cylinder pressure were obtained. Simulation results revealed that at 10% load conditions, with the increase of biodiesel blend ratio, the overall CO development and oxidation window is narrowed, and a remarkable increase in CO emission is observed.

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1. Introduction

Biodiesel has attracted extensive attentions around the world during the past few decades. It has been shown that the use of biodiesel creates cleaner combustion and reduced harmful emissions. Biodiesel fuels can be produced from vegetable oils or animal fats via trans-esterification process through which large molecule triglycerides are transformed into straight chain methyl esters with shorter carbon lengths to lower the viscosity of the fuel. Typical biodiesels derived from rapeseed oil, soybean oil or palm oil contain five major components of methyl esters with a carbon length of 17–19 which is still longer than conventional diesel fuel, thereby featuring an increased viscosity and may cause filter plugging and operating difficulties especially in cold climate applications [1]. Even though it can be directly utilized in diesel engines without any major modifications, biodiesel may still result in ring-sticking, injector coking, or injector deposits problems in the long run [2]. As such, in practical applications, biodiesel is seldom used in its neat form but blended with fossil diesel which is commonly labeled as a B factor "Bxx", where xx is the volume percentage of biodiesel.

Numerous studies have been conducted to experimentally evaluate the impacts of biodiesel blend ratio on the performance, combustion and emission characteristics of a diesel engine. It has been concluded that with the use of biodiesel, less carbon monoxide (CO), unburned hydrocarbon (UHC), and particulate matter (PM) emissions are observed [3,4]. The net carbon dioxide (CO_2) emission was also shown to be reduced since the growth of biodiesel feedstock (rapeseed, soybean or palm) consumed carbon dioxide during their lifetimes. Despite these environmental benefits, there are also some drawbacks with biodiesel that need to be overcome for a widespread application. The nitrogen oxides (NO_x)

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http://dx.doi.org/10.1016/j.apenergy.2014.01.004

Please cite this article in press as: An H et al. A numerical modeling on the emission characteristics of a diesel engine fueled by diesel and biodiesel blend fuels. Appl Energy (2014), http://dx.doi.org/10.1016/j.apenergy.2014.01.004

emission was reported to be slightly elevated by most of researchers. Many experimental studies have also shown that with biodiesel blend ratio increases, the brake specific fuel consumption (BSFC) increases [5,6]. This is mainly due to the presence of oxygen atoms in the biodiesel chemical structure, reducing its calorific value by 7–12%. The above mentioned studies mainly focused on the experimental characterization of the emission or performance indicators of a biodiesel fueled diesel engine. However, to better understand the underlying phenomena of the fuel oxidation and emission formation processes, three dimensional computational fluid dynamics (CFD) simulations are of critical importance.

Up to date, numerical modeling studies on biodiesel fueled diesel engine are still rare. This is presumably attributed to the lack of reliable biodiesel chemical kinetics with sufficiently small number of species and reactions that can be managed by a three dimensional workplace within an acceptable timeframe [7]. To reduce the overall size of the reaction mechanism, methyl butanoate (MB) was first proposed by Fisher et al. [8] as a surrogate fuel for biodiesel since it shares the same chemical structure of $RC(=O)OCH_3$. Although the carbon length of MB is much shorter than those of biodiesel methyl esters, it can still capture the fast RO_2 isomerization reactions which are important for the low temperature combustion chemistry that controls the fuel auto-ignition. To adjust for the fuel molecular weight and oxygen content, Brakora et al. [9] simulated soybean biodiesel with a two-component biodiesel mechanism, and it was assumed that biodiesel consisted of 1/3 of MB and 2/3 of n-heptane (C_7H_{16}) in mole. Based on a modified approach, Golovitchev and Yang [10] simulated a Volvo D12C diesel engine fueled by rapeseed methyl ester using a real biodiesel component: methyl linoleate ($C_{19}H_{34}O_2$) as the surrogate fuel. The developed mechanism comprises of 88 elementary species and 363 reactions, which combines the reaction mechanisms for three constituent components of MB, C_7H_{16} and toluene (C_7H_8O), with the soot and NO_x formation mechanisms embedded. To further include the large molecule dissociation and oxidation pathways, Herbinet et al. developed detailed reaction mechanisms for methyl decanoate (MD) [11], methyl-5-decenoate (MD5D) and methyl-9-decenoate (MD9D) [12], representing the saturated and unsaturated methyl esters. Later, based on these detailed mechanisms, Luo et al. [13] produced a tri-component surrogate mechanism for biodiesel which consists of MD, MD9D and n-heptane. The final skeletal mechanism consists of 115 species and 460 elementary reactions. A similar work was also done by Brokora [14], but a much smaller mechanism (69 species and 204 reactions) was obtained. To numerically evaluate the influences of biodiesel blend ratio, Um and Park [15] simulated a single cylinder diesel engine fueled by Diesel, B20 and B40 fuels with an injection pressure of 100 MPa and injection timing of −10° ATDC based on a reduced

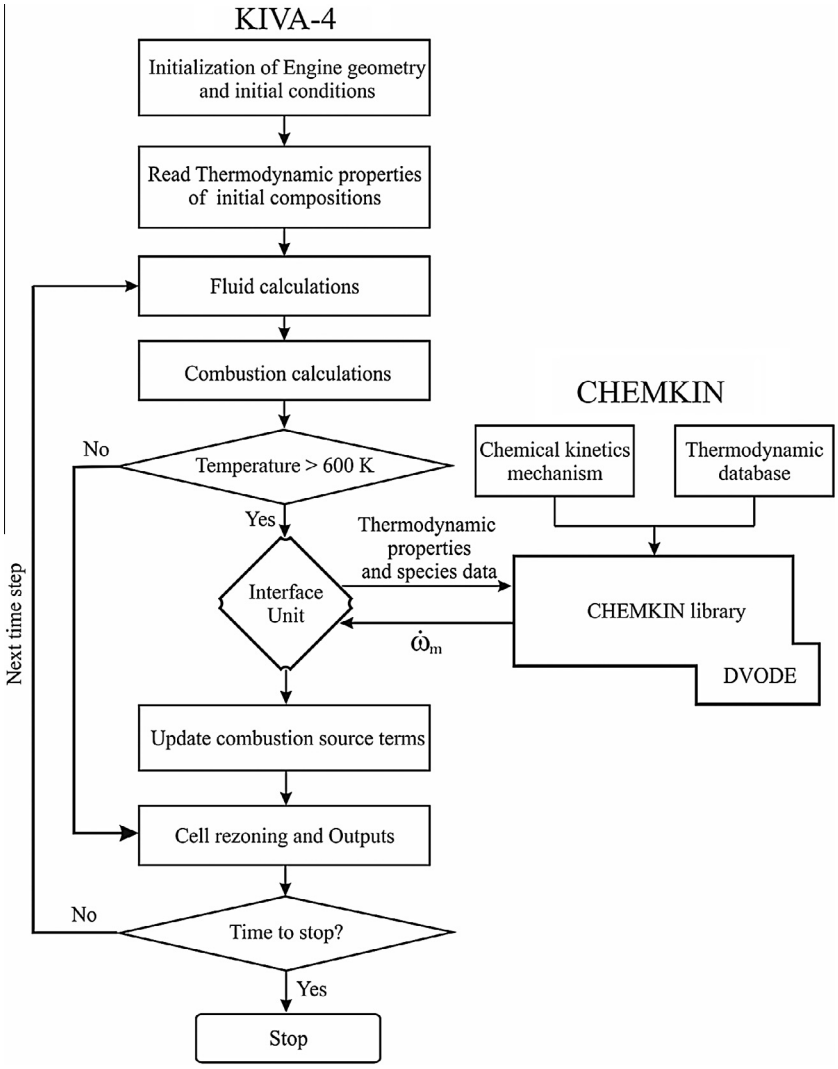

Fig. 1. Flow chart of integrated KIVA–CHEMKIN code.

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