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Effects of injection strategies and fuel injector configuration on combustion and emission characteristics of a D.I. diesel engine fueled by bio-diesel

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ABSTRACT

A multi-dimensional computational fluid dynamics (CFD) modeling was conducted on a D.I. (Direct Injection) diesel engine fueled by bio-diesel based on KIVA4 code. Comprehensive chemistry prediction of bio-diesel fuel was taken into account by enhancing the combustion model of the default KIVA4 code. An advanced multi-component fuel combustion model was applied to accurately predict the oxidation of saturated and unsaturated agents of the bio-diesel fuel using a reduced chemical kinetics mechanism. In order to accurately model spray, atomization and evaporation of the bio-diesel fuel, detailed thermo-physical properties of fuel components were predicted and tabulated in the fuel routine of the KIVA4 code. After the validation for cylinder pressure and heat release rate at engine mid load with experimental engine tests, further numerical studies were performed to investigate effects of injection strategies such as double and triple injection pulses and axial location of injector nozzle. It has been found that cylinder peak pressure was increased by applying double and triple injections and some enhancements on output power was also observed. Moreover, it was found that nozzle axial location has considerable effect on combustion of the bio-diesel fuel where wall impingement of the liquid bio-diesel fuel resulted in lower evaporation and higher unburnt hydro carbon (UHC) emission.

1. Introduction

Carbon dioxide and particulate matter (PM) as the major emissions have created serious air pollution problems around the globe. There have been yearly strengthened emission regulations on internal combustion engines to meet less emission levels. In this case, diesel engines are in spotlight as they carry on majority of burden in transportation such as trucks, buses and ships. Despite extensive researches on maximizing the efficiency and further reduce the emission levels, diesel engines still suffer from high soot and NO_x emission levels in variety of operating conditions and the degree of improvement seems to be not satisfactory. Over the past years, alternative fuels have been introduced and widely investigated as a promising solution for air pollution and fossil fuel shortage dilemma. Bio-diesel was seen as an alternative to conventional diesel due to its desirable attributes such as biodegradable, renewable, sustainable and carbon neutral [1]. It can directly replace petroleum diesel and be used in diesel engines without the requirement of any major modifications. In terms of emissions, researchers have shown that the use of bio-diesel can result in a substantial reduction in the unburned hydro-carbon (HC), PM and carbon monoxide (CO) emissions [2–4], even though a slight increase in nitrogen oxides NO_x emission is observed. Although engine experiments on bio-diesel fuels are essential tools to study, understand and optimize the typical compression ignition engines, the range of their applicability in terms of economy, time and available infrastructures is the matter of debate. Numerical simulations of internal combustion engines through detailed mathematical framework have been shown to be a very useful tool for saving experimental costs. 3D-CFD engine simulations consider temporal and spatial variations of the flow field, pressure, composition, temperature and turbulence inside combustion chamber and are much closer than thermodynamic models [5–7] to the real processes happening inside the combustion chamber. Nonetheless, the accuracy of dimensional models relies on the applied sub-models in the computational code. In case

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Abbreviations

ATDC	after top dead center
TDC	top dead center
BDC	bottom dead center
PM	particulate matter
CFD	computational fluid dynamics
KH-RT	kelvin helmholtz-rayleigh taylor
CO	carbon monoxide
MD	methyl decanoate
CO_2	carbon dioxide
MD9D	methyl-9-decenoate
D.I.	direct injection
SOI	start of injection
EVO	exhaust valve open

Symbol list

IC	internal combustion
CAD	crank angle degree
IVC	inlet valve closure
HRR	heat release rate
NO_x	nitrogen oxides
N_C	number of cylinders
SOI	start of injection
velinj	injection velocity

of bio-diesel combustion chemistry, one of the earliest attempts was done on methyl butanoate (MB) as a bio-diesel surrogate by Fisher et al. [8]. This is because MB possesses the essential chemical structural feature of the ester functional group. However, the carbon length of MB is much shorter than typical biodiesel methyl esters with chains of 16–18 carbon atoms, leading to a poor reproduction of the kinetic features of biodiesel fuels. Brakora et al. [9] developed reduced chemical kinetics mechanism for bio-diesel oxidation including MB as bio-diesel surrogate. They used combined MB/n-heptane mechanism in CFD calculations of the bio-diesel-fueled engine. Results of their modeling for pressure and heat release rate were in good agreement with experiments; however, NO_x emission was under-predicted for light engine load. Ng et al. [10] developed a multi-component chemical kinetics mechanism taking into account effects of saturated and unsaturated agents of bio-diesel fuel through using number of global reactions. They concluded that higher the amount of unsaturated fuel compounds, greater the combustion tendency to form acetylene and soot emission. Luo et al. [11,12] developed a skeletal mechanism with 115 species and 460 reactions for a tri-component bio-diesel surrogate consisting methyl decanoate, methyl 9-decanoate and n-heptane. The proposed mechanism was able to accurately predict ignition delay, flame lift-off length and equivalence ratio at flame lift-off location under different ambient conditions. They also validated their mechanism by using it as the governing chemistry in 3D turbulent spray combustion at compression ignition engine conditions.

It should be noted that comparing to conventional diesel fuel some of the important thermophysical properties of the bio-diesel fuels are noticeably different. Due to higher cetane number compared to diesel fuel most of the bio-diesel fuels have shorter chemical ignition delay time; however, number of researches [13–16] has shown that the physical ignition delay tends to increase by applying pure bio-diesel or its blend with diesel fuel. This is mainly due to higher kinematic viscosity and surface tension of the bio-diesel which cause longer time on bio-diesel fuel droplet evaporation. Due to such a change in fuel thermophysical properties, break up, atomization and evaporation of bio-diesel fuels take longer time and this has a direct effect on engine combustion and emission characteristics. This is the reason for injection strategy and timing being much more critical in bio-diesel driven engines comparing to diesel engine. In this regard, Qi et al. [17] experimentally investigated effects of injection timing and split injection with applying Exhaust Gas Recirculation (EGR). The engine experiment results showed that with retarding the main injection, brake specific fuel consumption was slightly increased, whereas NO_x emission was decreased. Moreover, they concluded that split injection strategy had less effect on soot emission. As it is mentioned, liquid fuel spray behavior of bio-diesel fuels is different from diesel due to different thermophysical properties. The main aim of this paper is to firstly introduce a reliable simulation workstation with detailed modeling of bio-diesel fuel properties and combustion, and secondly investigate the effects of injection strategies which were believed to have considerable effects on combustion and emission characteristics of a compression ignition engine fueled with bio-diesel.

2. Numerical simulation

2.1. 3D-CFD calculations

2.1.1. Fluid flow simulation

Compared to thermodynamic models, one of the main advantages of dimensional models is considering turbulent fluid flow effects. This is also done in thermodynamic models by introducing some correlations in applied governing equations; however, using these correlations, fluid flow is not modeled directly. In addition to this, large number of coefficients was needed to tune thermodynamic models which their values may not be valid in wide range of engine operating conditions. Nonetheless, there is a need to compromise accuracy with computational time in multi-dimensional simulation. Technically speaking, if the dimensional model would contain the detailed chemistry prediction, prolonged simulation time would be resulted. In the current study, KIVA4 is used as multi-dimensional CFD code. KIVA4 is a new version of KIVA code family [18] developed at Los Alamos National Laboratory (LANL) using Reynolds Averaged Navier–Stokes (RANS) method in modeling turbulent flow field and Arbitrary Lagrangian Eulerian (ALE) method for flow and liquid fuel spray simulations. KIVA is a well-recognized workstation for IC engine simulation task and a large number of researchers have used KIVA in simulations of combustion characteristics in a variety of IC engine operating modes [19–28]. Nevertheless, default KIVA code is not suitable in simulation of newly introduced alternative fuels such as bio-diesels for two main reasons. Firstly, fuel library of the KIVA code does not contain the thermophysical properties of different bio-diesel fuels and/or surrogate bio-diesel chemical species. Secondly, ignition and combustion calculations are based on a single-step global reaction of fuel oxidation to main products such as CO_2, CO and H_2O. This is a very unrealistic assumption as fuel ignition and process of combustion require breaking considerable C–H bonds and formation/dissociation of many intermediate chemical species. This phenomenon is more pronounced in bio-diesel fuels due to presence of variety of hydrocarbons with different molecular structure and thermochemical properties.