Applied Energy xxx (2016) xxx–xxx

Contents lists available at ScienceDirect

Applied Energy

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

Numerical analysis of spray characteristics of dimethyl ether and diethyl ether fuel

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HIGHLIGHTS

- Thermo-physical properties of liquid DME and DEE are reported.
- Ether fuels tend to cavitate higher compared to that of diesel fuel.
- Spray tip penetration and SMD are found to be lesser for ether fuels.
- Ether fuels shows excellent atomization behavior.

ARTICLE INFO

Article history:
Received 11 June 2015
Received in revised form 29 January 2016
Accepted 30 January 2016
Available online xxxx

Keywords:
Spray characteristics
Nozzle flow
Cavitation
DME
DEE

ABSTRACT

In this work, the spray characteristics of ether fuels such as dimethyl ether (DME) and diethyl ether (DEE) have been numerically investigated using KIVA-4 CFD code. A new hybrid spray model developed by coupling the standard KHRT model to cavitation sub model was used. The detailed thermo-physical properties of ether fuels have been predicted and validated with experimental results available from literature. The cavitation inception inside the injector nozzle hole has been studied for ether fuels in comparison with diesel fuel. It was found that ether fuels cavitates higher compared to that of conventional diesel fuel because of its low viscosity. The spray tip penetration of diesel fuel was longer than that of ether fuels due to high viscosity and density of diesel fuel. Ether fuels characterized by low Ohnesorge number and high Reynolds number showed better atomization behavior compared to that of the diesel fuel.

1. Introduction

Recent studies on compression ignition engines are focused on reduction of emissions such as oxides of nitrogen and particulate matters and find a suitable alternative for depleting fossil fuels. In order to suffice the objective, researchers are progressively studying on alternative fuels which can substitute conventional diesel and also help in reducing exhaust emissions. Among several alternative fuels, dimethyl ether (DME) and diethyl ether (DEE) are highly suitable fuel for compression ignition engines due to their excellent ignition quality because of higher cetane number than that of diesel, and low fuel based emissions due to their smaller carbon chains. Both DME and DEE are used in diesel engine either as sole fuel or blend fuel with diesel and are shown to be good replacement for diesel fuel both in terms of performance and emissions. Moreover DME has been recognized as neat fuel in the literature [1–3]. Wei et al. reported that particulate matter (PM) emissions decrease with engine speed and increase with engine load as the DME concentration increases in the diesel-DME blend fuel [4]. Park and Yoon investigated the effect of multiple injection strategy on DME fueled engine and found that both NO_x and soot reduced without deterioration to the engine performance compared to that of single injection [5]. Jeon et al. studied the difference in combustion of ULSD and DME in optical single cylinder engine and reported that the DME combustion is characterized by faster burning rates and higher peak combustion pressure compared to that of ULSD. They also reported that DME combustion exhausted extremely small quantities of soot in all engine test conditions whereas ULSD showed very high levels of soot emissions [6]. In order to increase the use of DME in internal combustion engines, a novel common rail injector was developed at State Key Laboratory of Engines, China. This injector had an advantage of opening response not affected by the common rail pressure which is very common in using diesel common rail injector for DME

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http://dx.doi.org/10.1016/j.apenergy.2016.01.128
0306-2619/

fuels [7]. DEE has been reported to be used as additive to improve the cold starting performance due to its high cetane number (approximately 125) [8]. DEE also has an advantage over DME as it exists in liquid phase under atmospheric conditions and can be effectively blended with diesel and biodiesel fuels [9–13]. Polat studied the effect of diethyl ether, ethanol and diesel blend on HCCI combustion and found that blend fuel yielded almost zero NO_x emissions and also improved HCCI combustion, engine performance and exhaust emissions [14]. Ali et al. studied the effect of blending diethyl ether to biodiesel-diesel blend (B30) and found that the addition of diethyl ether improves the properties of the blended fuel, however, worsens the heating value and increases the cyclic variations slightly [15]. Tudu et al. studied the effect of diethyl ether in DI engine fueled by tyre derived fuel-diesel blend and reported that addition 4% DEE improved the brake specific fuel consumption by 6% and reduced NO emissions to 25% compared to that of diesel fuel operation at full load [16]. However there are still more potential to make it a complete or partial replacement to fossil fuels which require extensive optimization and series of experiments. In order to avoid extensive experiments, CFD comes handy for the purpose.

Cavitation and turbulence inside the injector nozzle hole play a significant role in primary spray breakup and development process [17]. The cavitation phenomenon differs for different fuels as they have distinct properties like vapor pressure, viscosity, density and surface tension. Hence it is very important to understand the internal nozzle flow of ethers like DME and DEE and their effect on spray evolution inside the combustion chamber. It was reported that high vapor pressure and lower viscosity of DME fuel can cause cavitation inception in the injector nozzle holes. This frequent cavitation occurrence and change in physical state can cause poor spray tip penetration inside the combustion chamber causing local high equivalence ratio region leading to high NO_x and CO emissions [18]. Thus, the study of cavitation behavior of ether fuels is important to understand its effect on spray characteristics. Availability of very few studies on modeling spray atomization of ether fuels taking into account the nozzle flow characterization provided motivation for the present work.

This study is focused on numerical investigation of the cavitation characteristics of ether fuels and its effect on spray development process. To simulate the spray characteristics of ether fuels, the detailed liquid thermo-physical properties should be known. Teng et al. [19] have predicted the liquid thermo-physical properties for DME fuel using various prediction methods available in literature. However, there is no literature for thermo-physical properties of DEE fuel. The prediction methods proposed in this work complements Teng et al. [19] for DME fuel and reports properties of DEE fuel for the first time in literature. Then, the cavitation behavior of ether fuels have been studied numerically using Fluent 13.0 CFD software and compared with that of diesel fuel. Finally, the spray characteristics of ether fuels have been investigated using a new hybrid spray model incorporated in multi-dimensional engine CFD code KIVA-4.

2. Methodology

2.1. Numerical simulation

The cavitation study was carried out using Fluent 13.0. The two-phase model by Schnerr and Sauer was used in this study to simulate the cavitation flow inside the injector nozzle holes. For spray modelling, a new hybrid model developed by the authors is used. The spray model is developed by coupling the cavitation sub model to the classical KH-RT model. In the new model, the dominant spray breakup process is determined by the maximum of length to time scale ratio. The mathematical form of the new hybrid model is given in Eq. (1) [20,21]

$$\frac{L_B}{\tau_B} = \max\left\{\frac{L_{KH}}{\tau_{KH}}, \frac{L_{RT}}{\tau_{RT}}, \frac{L_{cav}}{\tau_{cav}}\right\} \quad (1)$$

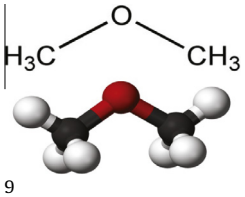
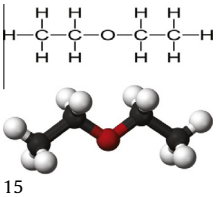
where L is the characteristic length and τ is the characteristic time and the subscripts B, KH, RT, cav represent dominant break-up process, Kelvin–Helmholtz (KH) model, Rayleigh–Taylor (RT) model and cavitation model respectively. The parameters like average turbulent kinetic energy, area coefficient, coefficient of discharge and vapor volume fraction are obtained from the results of local distribution of flow field variables in the nozzle exit through internal nozzle flow simulations. Then these parameters are keyed in as input to the new hybrid spray model to capture the effects of turbulence and cavitation in spray development process to improve the primary atomization process. The model was implemented into KIVA-4 using a separate sub-routine written in FORTRAN language. For further details on the model please refer to Mohan et al. [20].

3. Results and discussion

3.1. Prediction of thermo-physical properties

The default KIVA-4 fuel library has only gaseous thermo-physical properties of DME and does not include properties of DEE. In order to include the liquid properties of both DME and DEE, it should be first predicted over a range of temperature since experimental values are available only at certain temperatures. The

Table 1
Critical properties of DME and DEE.

	Dimethyl Ether (DME)	Diethyl Ether (DEE)
Molecular weight	46.684	74.1216
Molecular structure		
No of atoms	9	15
Critical temperature	401 ± 2 K	467 ± 2 K
Critical pressure	54 ± 3 bar	36 ± 1 bar
Boiling point	249 ± 1 K	307.7 ± 0.2 K

Please cite this article in press as: Mohan B et al. Numerical analysis of spray characteristics of dimethyl ether and diethyl ether fuel. Appl Energy (2016), http://dx.doi.org/10.1016/j.apenergy.2016.01.128