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Numerical simulation on spray characteristics of ether fuels

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Abstract

In this study, the spray characteristics of ether fuels have been studied numerically using a new hybrid spray model in KIVA4 CFD code which accounts for cavitation inside he injector nozzle holes. The cavitation phenomenon was investigated numerically using Fluent CFD software. The properties of ether fuels have been predicted and reported. It is found that ether fuels cavitates higher compared to diesel fuel which means high fuel quantity should be injected to achieve same power output as diesel fueled engine. The spray simulation shows the atomization of ether fuels are far superior to diesel as they are characterized by high Reynolds number and low Ohnesorge number.

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Keywords : spray characteristics, nozzle flow, cavitation, DME, DEE, ethers

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 diesel, and low fuel based emissions due to their smaller carbon chains. Both DME and DEE are used in diesel engine as sole fuel and also as blend fuel with diesel and were 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].

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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 plays a significant role in primary spray breakup and development process [4]. The cavitation phenomenon differs with different fuel 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. Thus, this study is focused on numerical study of the cavitation characteristics of ether fuels and its effect on spray development process.

2. Methodology

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 equation below [5]

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

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.

3. Results and discussion

3.1. Prediction of thermo-physical properties

The default KIVA4 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 properties like vapor pressure, density, latent heat of vaporization, viscosity, surface tension and thermal conductivity are required to model the spray dynamics of DME and DEE. In order to ensure the accuracy of modeling, the accurate prediction of these properties is significant. There are many methods in predicting the properties, however the methods used in this study predicts the properties in good agreement with the experimental data available in literature (shown in Table 1). The properties are predicted based on the critical temperature, critical pressure, boiling point, molecular weight and molecular structure of DME and DEE. The predicted properties of DME and DEE are shown in Fig.1 in comparison with diesel.

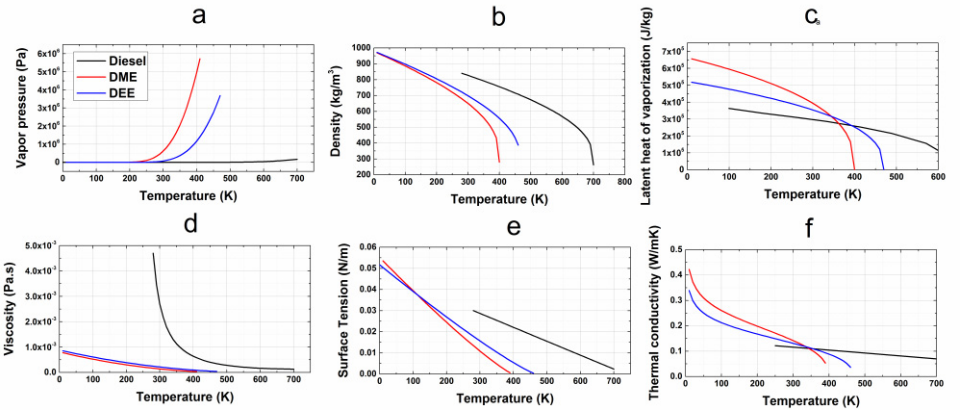

Fig.1. Comparison of vapor pressure, density, latent heat of vaporization, viscosity, surface tension and thermal conductivity of DME and DEE with diesel

Table 1. Prediction methods for different properties

Properties	Prediction method [6]		Experimental value		Predicted value	
	DME	DEE	DME	DEE	DME	DEE
Vapor pressure	Antoine's equation	Taylor and Smith	Boiling point at 1atm 249K	Boiling point at 1atm 307.7K	Boiling point at 1 atm 248.1K	Boiling point at 1atm 307.4K
Density	modified Rackett equation	modified Rackett equation	at 293K - 0.66g/cc	at 293 K - 0.7133g/cc	at 293K - 0.661g/cc	at 293 K - 0.7112g/cc
Latent heat of vaporization	Pitzer accentric factor	Pitzer accentric factor	at 248.34K - 21.51 kJ/mol	at 307.6K – 26.52kJ/mol	at 248.34K - 21.20 kJ/mol	at 307.6K – 26.51kJ/mol
Viscosity	Letsou and Stiel	Letsou and Stiel	at 298K - 0.15cP	at 298K - 0.224cP	at 298K - 0.143cP	at 298K - 0.2198cP
Surface tension	Brock and Bird correlation	Brock and Bird correlation	at 298 - 11.731dyne/cm	at 298 – 16.47dyne/cm	at 298 - 11.12dyne/cm	at 298 – 15.9dyne/cm
Thermal conductivity	Latini et al.	Latini et al.	at 234K - 0.1456, W/mK	na	at 234K - 0.1551 W/mK	na

3.2. Experimental results and validation of model

Fig.2 shows the comparison of spray tip penetration between experimental [7] and simulation results at injection pressure of 50 and 100MPa under ambient pressure of 3 and 6Mpa for diesel fuel. The spray tip penetration at injection pressure of 100MPa is longer compared to 50MPa; this is because of the higher injection velocity and spray momentum attributed by higher injection pressure. It should also be noted that for same injection pressure, as the ambient pressure increases from 3 to 6MPa, the spray tip penetration decreases; this is because of the fact that at higher ambient pressure; the spray loses its momentum energy faster which results in shorter penetration length.

These complete spray characteristics were captured well by the new hybrid model. This shows that the new hybrid model is capable of predicting the spray characteristics accurately.

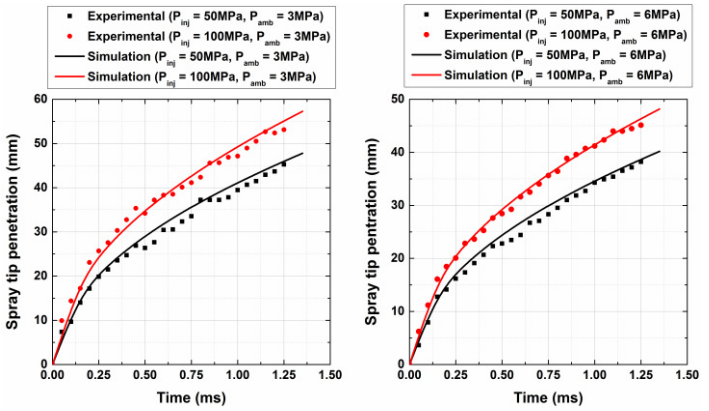

Fig. 2. Comparison between experimental and simulation results of spray tip penetration at various ambient pressures for diesel fuel

3.3. Nozzle flow simulation

The nozzle flow simulations were carried out for different injection pressure (50, 100 and 150MPa) under different ambient pressure conditions (3 and 6MPa). The thermo-physical properties like vapor pressure, viscosity, density and surface tension found earlier were used in the simulations. Fig.3 presents the cavitation inception of diesel, DME and DEE fuels inside the injector nozzle hole under ambient pressure of 6MPa and varying injection pressures. From Fig.3, it is clear that the cavitation increases with the increasing injection pressure, this is due to the fact that with increasing pressure difference, the turbulence inside the nozzle increases and subsequently increases the cavitation inception. Also it should be noted that the DME cavitates higher followed by DEE and diesel fuel. This is mainly due to the differences in their viscosity. As DME possesses very less viscosity (refer to Fig.1d), it has high Reynolds number under same injection and ambient pressures than DEE and diesel, which in turn creates high amount of turbulence inside the nozzle hole and eventually leading to higher cavitation. Also it should be noted that the vapor pressure of DME is very high compared to DEE and diesel (refer to Fig.1a), which also increases the tendency of DME cavitation.

Fig.4a shows the mass flow rate and discharge coefficient of DME, DEE and diesel under different pressure difference. It should be noted that the mass flow rate of DME is lesser followed by DEE and diesel, this is because, DME and DEE has higher cavitation and lesser density compared to diesel fuel. The cavitation plays an important role in lesser mass flow rate of ethers, which is evident from the discharge coefficient of DME and DEE, as it is lesser than diesel fuel, because of higher vapor formation that extends to the outlet of the nozzle (refer Fig.3). This shows that when pure DME or DEE used as an alternative to diesel fuel in engine without any modification to injection duration then it is very obvious that the engine gets lesser fuel compared to diesel injection. Less mass flow rate along with less calorific value of DME and DEE compared to diesel will generate lesser power when directly used as substitutes. This phenomenon was also observed by other researchers when DME is used in engines, it required longer injection duration to meet power requirement compared to diesel [2]. Fig.4b shows the comparison of injection velocity between diesel fuel and ethers. Ethers possess higher injection velocity than diesel

fuel due to their less viscous nature. The less viscosity of ethers ensures less viscous loss in flow which increases the flow momentum and hence increases the exit velocity. This increase in injection velocity helps in better atomization of ethers compared to diesel.

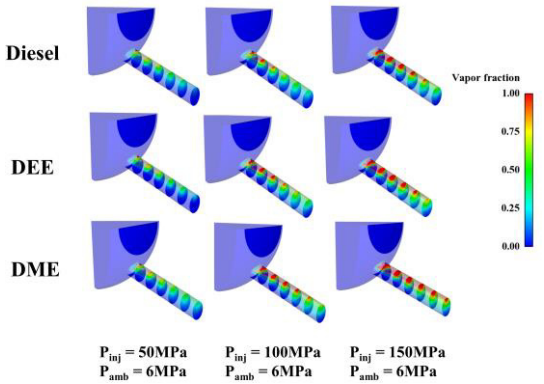

Fig.3. Comparison of cavitation inception with different fuels under different injection pressures

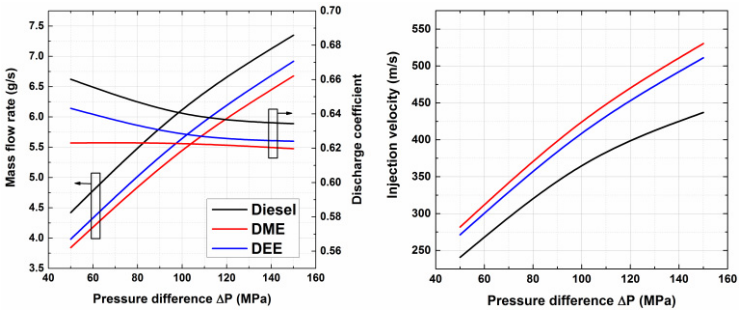

Fig. 4. (a) Mass flow rate and; (b) injection velocity of different fuels under different pressure difference

3.4. Spray simulation

Fig.5a shows the spray tip and SMD comparison between diesel, DME and DEE fuels. The spray penetration of diesel fuel is comparatively longer than ether fuels. This is due to high viscosity and density possessed by diesel. Similarly DEE shows longer penetration than DME for the same reason. The droplet size decreasing rate for ethers are much higher because of various properties like low viscosity, high vapor pressure and low surface tension. Nevertheless, the droplet size of DEE is higher compared to DME because of its relatively higher surface tension. Fig.5b shows the atomization behavior of different fuels on Ohnesorge diagram [8]. It should be noted that though atomization of diesel and ether fuels behave similarly i.e. they fall on atomization regime, the level of atomization differs between them. Ether fuels are atomized better since they are characterized by higher Reynolds number and lower Ohnesorge number compared to diesel for same injection pressure. High Reynolds number signifies high turbulence and aerodynamic forces on droplets which help in finer droplet formation. Also lower Ohnesorge number signifies low viscosity and low surface tension which means smaller droplet sizes. Hence this diagram shows that ether fuels exhibits excellent atomization behavior compared to diesel fuel, which will help in better air fuel mixing and ensures clean and proper combustion.

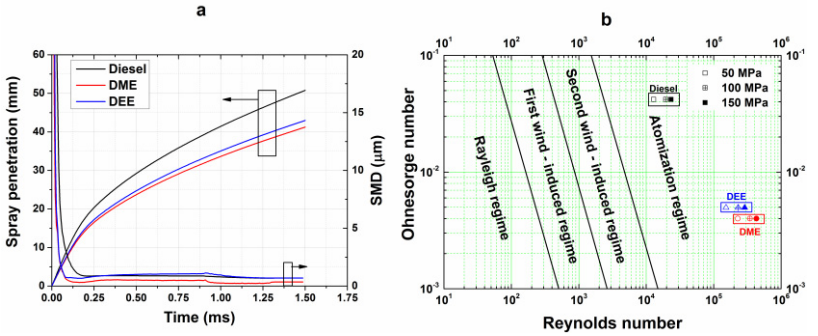

Fig.5. (a) Spray tip penetration and SMD comparison between diesel and ether fuels; (b) Ohnesorge diagram

4. Conclusions

The properties of ether fuels have been predicted and reported. The ether fuels show high level of cavitation compared to diesel. However, DME and DEE exhibit excellent atomization behavior compared to diesel fuel.

Acknowledgements

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Biography

Balaji Mohan is a PhD student at the National university of Singapore. His research interests are fuel spray, two phase flow and combustion with emphasis on experimental analysis and mathematical modeling.