Applied Thermal Engineering 159 (2019) 113909

Contents lists available at ScienceDirect

Applied Thermal Engineering

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

Research Paper

Effect of toluene content on the combustion and emissions of large two-stroke marine diesel engine

Xiuxiu Sun[a], Xingyu Liang[b,*], Gequn Shu[b], Yuesen Wang[b], Yong Chen[a]

[a] School of Mechanical Engineering, Hebei University of Technology, Tianjin 300401, China
[b] State Key Laboratory of Engines, Tianjin University, Tianjin 300072, China

HIGHLIGHTS

- The simulated results of marine diesel engine were validated.
- The engine combustion characteristics of four surrogate fuels were investigated.
- The effects of different liquid properties were investigated.
- The optimal surrogate fuel was proposed for the marine diesel fuel.

ARTICLE INFO

Keywords:
Toluene
Surrogate fuel
Computational fluid dynamics
Marine diesel engine

ABSTRACT

A computational fluid dynamics (CFD) simulation model has been established to study the effects of toluene content in surrogate fuel on combustion and emissions for a large two-stroke marine diesel engine. In order to find more accuracy simulation model, the effects of toluene physical parameters were researched. Meanwhile the paper suggests a multi-components mechanism as surrogate fuel of diesel. The results indicate that the toluene content in surrogate fuel has an important impact on performance of marine engine. The ignition delay times increases with an increase in toluene content. However, the nitrogen oxide and soot mass are increase. The combustion will be influenced when the physical parameters of toluene are used in liquid fuel mixture. The nitrogen oxide has a peak value when the toluene content is used in the liquid fuel mixture. However, it has little influence on the in-cylinder pressure. The liquid parameters have also effect on the accuracy of simulation model. The in-cylinder pressure and emissions are higher when *n*-tetradecane is used in the liquid fuel mixture. By comparing the key parameters determined from simulations and experiments, it is found that the *n*-tetradecane-toluene with 30% of toluene is applicable to use as surrogate fuel of diesel.

1. Introduction

The introduction and enforcement of stringent environmental regulations has made it necessary for engine manufacturers to produce marine diesel engines with lower exhaust emissions. According to the International Marine Organization Tier III regulations, nitrogen oxide (NO_x) emissions need to be reduced from 14.4 g/kWh (Tier II regulations) to 3.4 g/kWh [1]. Various techniques have been developed over the years to produce marine diesel engines that fulfil this requirement such as exhaust gas recirculation (EGR), selective catalytic reduction (SCR) and humid air motors (HAMs) [2–4]. Numerical simulations are now widely used to simulate the performance and exhaust emissions of marine diesel engines with advances in computer technology and software.

Compared with real-world testing, numerical simulations are used to investigate the performance and exhaust emissions of marine diesel engines over a wide range of conditions while reducing significant resources and time associated with conventional experimentation. Ji et al. [5] researched the effects of Miller cycle, exhaust gas recirculation and intake air humidification coupled with fuel injection strategies on the NO_x emissions using CFD software CONVERGE. A CTC/SHELL model was used to simulate auto-ignition of fuel. The surrogate fuel and combustion model were also used by Jiang et al. to research the effects of multiple-Injection coupled with EGR on combustion and NO_x emissions in a marine diesel engine [6]. Zhou et al. [7] investigated the effect of injection direction and exhaust valve close timing on performance and emissions for a slow speed marine engine. The multi-zone sub-model was selected in combustion model. Sigurdsson et al. [8]

* Corresponding author.
E-mail address: lxy@tju.edu.cn (X. Liang).

https://doi.org/10.1016/j.applthermaleng.2019.113909
Received 9 November 2018; Received in revised form 27 May 2019; Accepted 2 June 2019
Available online 03 June 2019
1359-4311/

developed a novel CFD model to study the scavenging process and convective heat transfer of a large, two-stroke low-speed uniflow-scavenged marine diesel engine. The combustion model is an important part for number simulations. The choosing of combustion model has relationship with the chemical kinetics of surrogate fuels. For this reason, the studies on surrogate fuels are one of the key areas of combustion research.

Alkanes are typically used as diesel surrogate fuels, including heptane [9], dodecane [10] and tetradecane [11]. Pang et al. [12] studied the soot formation and oxidation process of a two-stroke marine diesel engine where *n*-heptane was used as the diesel surrogate fuel. The mechanism consisted of 30 species and 68 reactions. The peak pressure determined from simulations was lower than that from experiments by 1.7%. Stratsianis et al. [13] used *n*-heptane as the surrogate fuel in a marine diesel engine and investigated the effect of post-injection on the engine performance and pollutant emissions. Kontoulis et al. [14] studied the effects of advanced injection strategies on the NO_x and soot emissions of a marine diesel engine where tetradecane was used as the surrogate fuel. Lamas et al. [15] researched the effects of multiple injection strategies on emissions and performance in the Wärtsilä 6L 46 marine engine. The model of *n*-heptane was employed to characterize the combustion kinetics. Based on these studies, single alkane components are often used as diesel surrogate fuels for the marine diesel engine. Mechanisms have been developed over the years, including detailed and simplified single-component mechanisms [16–18]. However, single-component surrogate fuels do not reproduce well the ignition characteristics of diesel fuel, the importance of the multi-components has been more concerned by researchers [19].

The composition of commercial diesel fuel was intrinsically complex [20]. The high aromatic content of diesel fuel leads to low reactivity of the fuel and increases the formation of PAHs. Some researchers have proposed using mixtures of alkanes and aromatics as diesel surrogate fuels [21]. Barths et al. [22] found that the two-component IDEA fuel (70% of *n*-decane + 30% of α-methylnaphthalene) has properties similar to those for diesel fuel. There is good agreement in the experimental results between the two-component IDEA fuel and diesel throughout the entire combustion cycle in terms of the ignition delay, maximum pressure, engine torque and pollutant formation. Andrae et al. [23] developed a semi-detailed mechanism (consisting of 137 species and 633 reactions) for autoignition of toluene-based reference fuels. Skeletal mechanisms for iso-octane and *n*-heptane were added to the detailed toluene sub-mechanism. Experiments have been carried out in recent years using homogeneous charge compression ignition (HCCI) engines fueled with toluene-based fuels in various operating conditions. These results were compared with those from simulations and other experimental studies in order to determine the correlation between ignition delay and empirical measurements of the autoignition quality of toluene-based fuels. Javed et al. [24] studied the ignition delay time of four ternary blends of *n*-heptane, iso-octane, and toluene, which were labeled as Toluene Primary Reference Fuels (TPRFs). The results showed that the kinetic model needs to be further improved in order to enhance the accuracy of predictions at low-temperature conditions, particularly, for highly sensitive TPRF blends with high concentrations of toluene.

Previous studies have also shown that the toluene content of surrogate fuels has a significant effect on the performance and exhaust emissions of diesel engines. Wang et al. [25] investigated the effect of toluene reference fuels (TRFs) with 15% and 30% of toluene on the combustion characteristics of diesel engine. They proposed a reduced mechanism (consisting of 109 species and 543 reactions) to represent the combustion chemistry of the TRFs (*n*-heptane, iso-octane and toluene) and PAHs in order to simulate the combustion process and the formation of PAHs and soot. The results showed that increasing the toluene content of the TRFs significantly increases the formation of PAHs and soot. However, the TRFs result in improved mixing due to longer ignition delay, which promotes soot oxidation and, leads to lower soot emissions compared with those for diesel. Liu et al. [26] developed and validated a reduced *n*-dodecane-TRF-c-hexane-PAH mechanism for diesel surrogate fuels. They formulated three potential diesel surrogate fuels have been performed: (1) 85% of *n*-heptane + 15% of toluene, (2) 81% of *n*-heptane + 14% of toluene, and (3) 5% of c-hexane + 80% of *n*-heptane + 20% of toluene. Zhang et al. [27] researched the combustion characteristic of diesel using number simulation. A reduced oxidation mechanism for diesel surrogate fuel based on *n*-heptane and toluene was developed, which consists of 60% *n*-heptane and 40% toluene by mass. In general, based on the results of previous studies, the use of toluene as a representative aromatic compound in the surrogate fuel increases the accuracy and reliability of the reaction mechanisms used to model the combustion process of diesel fuel. However, the effects of toluene content in surrogate fuel are unclear on the performance of marine diesel engine. The physical properties of toluene have relationship with the spray quantity of fuels. It is necessary to research the influences of toluene physical parameters. The accuracy of simulations can be improved by using the applicable toluene content in surrogate fuel and liquid model.

In this study, four diesel surrogate fuels were formulated. Three liquids were used to model the physical properties of diesel used in marine diesel engine. The effects of toluene content are investigated on the performance of marine diesel engine. The surrogate fuel was proposed by comparing the errors of the key parameters obtained from simulations with those from experiments. This study offers an in-depth insight on the surrogate fuel used to simulate the combustion process in marine diesel engines, which will improve the accuracy of CFD simulations.

2. Numerical model

CFD simulations of marine diesel engine (6S35ME-B9) described in a previous paper [28]. To more accurately simulate high Reynolds number in cylinder, the RNG k-ε sub-model was chosen as Reynolds Averaged Navier-Stokes (RANS) turbulence model in this paper [7]. The Kelvin Helmholtz-Rayleigh Taylor model is applied to the simulation of spray breakup. The atomization process of a diesel engine is a complex gas-liquid two-phase flow process. The KH mode is used to describe the breakup phenomenon in a liquid-core zone. In the gas-liquid mixing zone, the process of droplet breakup is described with both the KH and RT model. The No Time Counter (NTC) collision model is implemented to simulate the fuel collision. The NTC method is based on techniques used in gas dynamics for Direct Simulation Monte Carlo (DSMC) calculations. This model has been shown to be faster and more accurate than O'Rourke's model under certain conditions [29]. The droplet coalescence is used in the O'Rourke model based on Weber number, film thickness and viscosity [30]. The detailed chemical kinetics model SAGE is selected in combustion model. The detailed chemical kinetics is used in combustion simulation. The SAGE model calculates the reaction rates for each elementary reaction while the CFD solves the transport equations [31]. The *n*-tetradecane-toluene chemical mechanism is obtained from the published paper [32]. Finally, an Extended Zeldovich NO_x model and the Hiroyasu soot model are implemented to predict NO_x emission and simulate soot production [33]. The technical specifications of the marine diesel engine are presented in Table 1. The injection duration is 15.36°CA and the total injection mass is 0.0126 kg, which are obtained from the experimental data.

3. Validation of the numerical model

The engine speed and power are 142 rpm and 3575 kW, respectively, at full load. The experiment was down at Shanghai Maritime University. The in-cylinder pressure and emissions at the exhaust manifold were measured to validate the accuracy of the numerical model. Fig. 1 shows the comparison of the in-cylinder pressure between the simulation and experiments and it can be seen that there is good

Table 1
6S35ME-B9 test engine specifications.

Structure parameter	
Cylinder number	6
Bore (mm)	350
Stroke (mm)	1550
Displacement (L)	149
Compression ratio	21
Connecting rod length (mm)	1550

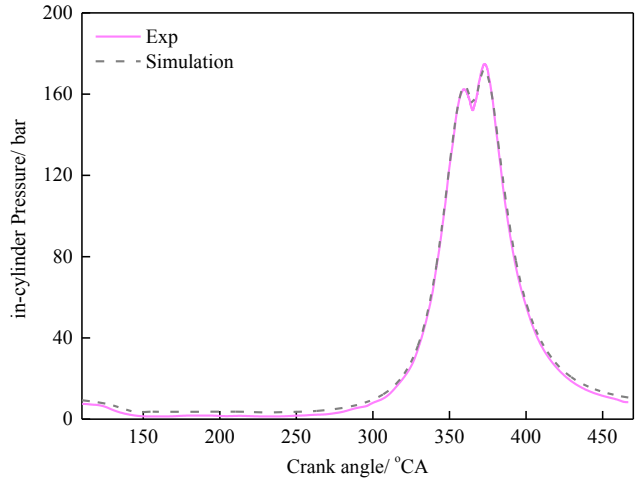

Fig. 1. Comparison of in-cylinder pressure for the simulation and experimental values.

agreement between the simulation and experimental values. The maximum in-cylinder pressure error during the combustion phase is 1.5% relative to the experimental values. The ignition delay is shorter by 0.8 °CA advanced compared with that from experiments. These errors are considered to be acceptable.

The emissions are important parameters to validate the accuracy of simulation model. The NO_x and carbon dioxide (CO_2) emissions obtained from simulation and experiment were compared, as shown in Fig. 2. The error between the simulation and experimental values for NO_x is 2.2%. The CO_2 emissions from simulation are lower than those from experiments. The error is more pronounced for CO_2 emissions compared with that for NO_x emissions because of, the combustion process. This is due to the fact that a reduced single-component (*n*-tetradecane) mechanism was used to simulate the combustion process

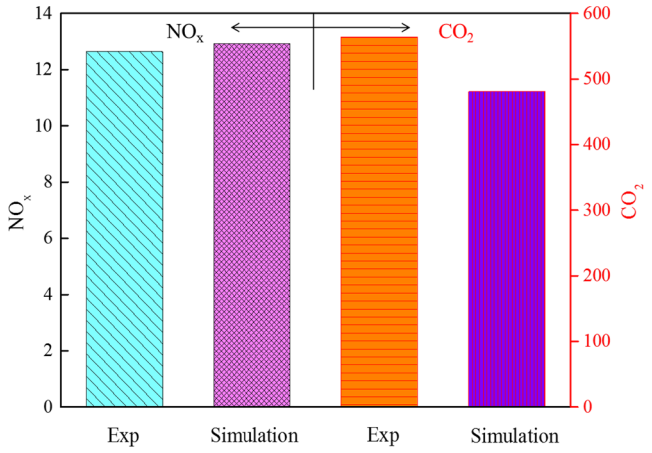

Fig. 2. Comparisons of NO_x and CO_2 for the simulation and experimental values.

in order to reduce the computational time. This reduced mechanism eliminates some of the CO_2-producing reactions, resulting in a larger error for the CO_2 emissions. In general, it can be deduced that the numerical model is capable of predicting the NO_x emissions with reasonable accuracy and therefore, the numerical model was used to examine the effect of different surrogate fuels on the combustion characteristics and exhaust emissions of the marine diesel engine. The simulation results were then compared with those from experiments.

4. Results and discussion

4.1. Comparison of the in-cylinder pressures for surrogate fuels with the same liquid properties

The effects of four surrogate fuels with the same liquid properties were investigated in this study: (1) 85% of *n*-tetradecane + 15% of toluene, (2) 70% of *n*-tetradecane + 30% of toluene, (3) 55% of *n*-tetradecane + 45% of toluene, and (4) 40% of *n*-tetradecane + 60% of toluene. The surrogate fuels include two species: *n*-tetradecane and toluene. The percent is the mass fraction. The surrogate fuels have different chemical composition, which are used in CFD model to obtained suitable surrogate fuel by compared with the experimental data. The experimental data is obtained from the Section 3. The properties of diesel were used in the parcel simulations of CFD model. The injection mass, time, rate, and duration were kept constant. The named of simulation cases are shown in Table 2.

Fig. 3 shows the comparison of the in-cylinder pressures of the surrogate fuels with different toluene content. The *n*-tetradecane was used as surrogate fuel in the 0% toluene case. It can be observed that the toluene content has large effect on the ignition delay times of fuels. The ignition delay gradually increases with an increase in toluene content. The ignition times of the surrogate fuel with 60% toluene from simulation delay nearly 1.5 °CA compared with the results using the surrogate fuel with 15% toluene. The ignition times of combustion reaction is depended on the mechanisms of *n*-tetradecane and toluene. The oxidation reactions of *n*-tetradecane and toluene are different, which is shown in Fig. 4. The ignition delay times of toluene is longer than that of *n*-tetradecane due to the reaction rate and activation energy of elementary reaction. However, the large quantity of OH are produced by combustion reaction of toluene due to the reaction of $C_6H_5CH_2$ and HO_2. The more fuel are consumed, which makes the rate of combustion reaction increasing. The maximum in-cylinder pressure increases with an increase in toluene content.

The results are compared with the experiment data to find a suitable surrogate fuel for simulations. It is found that there is a small error in the ignition delay between simulations and experiments for surrogate fuels with 30% and 45% of toluene. However, the error of maximum in-cylinder pressure is largest for the surrogate fuel with 30% of toluene compared with experimental data, which is about 2%. The in-cylinder pressure errors are considered to be acceptable for the surrogate fuel used in the simulations. However, it is not possible to identify the appropriate surrogate fuel based on the results of in-cylinder pressure.

Table 2
The named of simulation cases.

Liquid data	Surrogate fuels		Named
	n-tetradecane (C14H30)	Toluene (C7H8)	
Diesel	85%	15%	15% toluene
Diesel	70%	30%	30% toluene
Diesel + C7H8	85%	15%	Diesel + C7H8 15%
Diesel + C7H8	70%	30%	Diesel + C7H8 30%
C14H30 + C7H8	85%	15%	C14H30 + C7H8 15%
C14H30 + C7H8	70%	30%	C14H30 + C7H8 30%

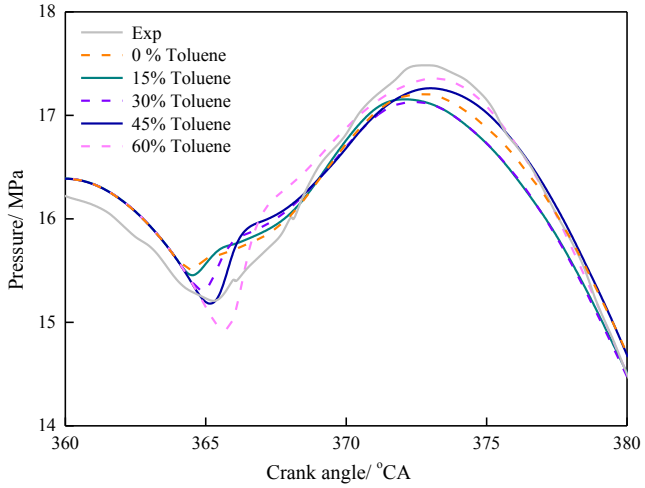

Fig. 3. Comparison of in-cylinder pressures for the different surrogate fuels.

Fig. 5 shows the comparison between the simulation and experimental values for engine power and brake specific fuel consumption (BSFC). The indicated power was determined from the simulation results. The net output power of crank is named as effective power. The fuel injection mass of simulations was set based on the experimental data. The indicated specific fuel consumption (ISFC) was determined by dividing the fuel injection mass flow rate with the indicated power. The effective power and BSFC were determined from the mechanical efficiency. The power decreases with an increase in toluene content. The pressure decreases with the increasing of toluene content due to the ignition times of combustion reaction delay. The power is proportional to in-cylinder pressure. The positive work of engine reduces. However, the injection mass are constant for simulations. The trends of BSFC are opposite with the changes of power. It is found that the effective power of the surrogate fuel with 30% of toluene determined from simulations is closest to that from experiments, where the ratio between the simulation and experimental values is 0.997.

The in-cylinder pressure, effective power and BSFC are the key parameters used to gauge the performance of the marine diesel engine. In general, the errors of these key parameters are considered to be acceptable. The key parameters determined from simulations are closest to the experimental values for the surrogate fuels with 30% and 45% of toluene.

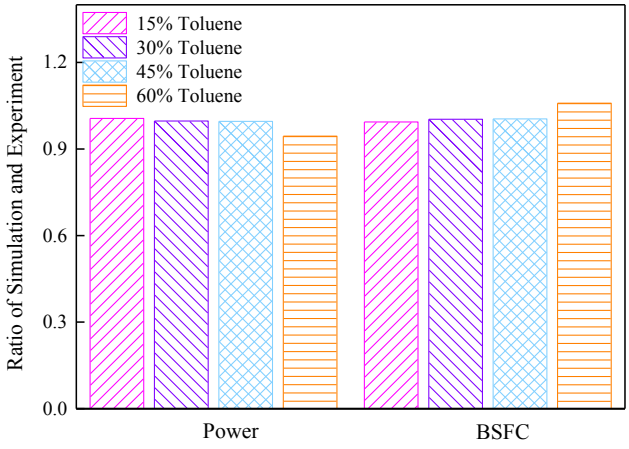

Fig. 5. Comparisons of power and BSFC for the different surrogate fuels.

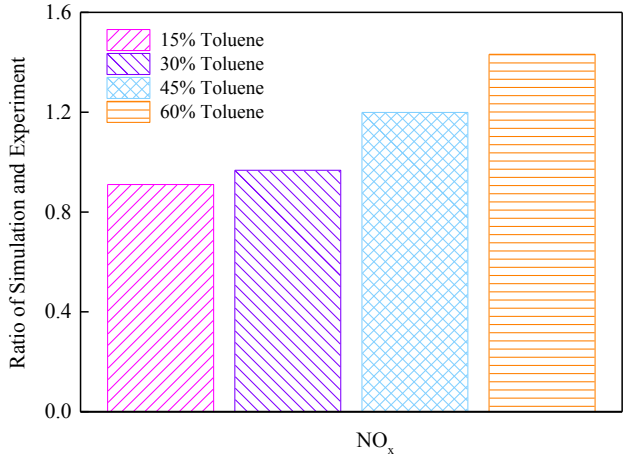

Fig. 6. Comparisons of NO_x emissions for the different surrogate fuels.

4.2. Comparison of the exhaust emissions for surrogate fuels with the same liquid properties

Fig. 6 shows the comparison of the NO_x emissions of the surrogate fuels with different toluene content. The NO_x emissions increase with an increase in toluene content. The extended Zeldovich mechanism is given by the following set of reactions:

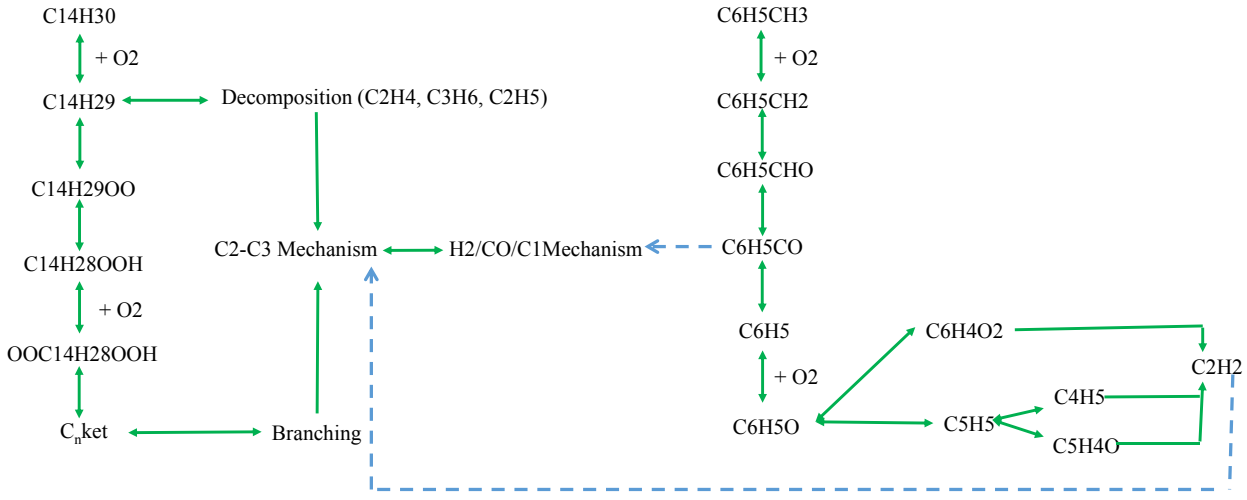

Fig. 4. Major reaction branches of *n*-tetradecane and toluene oxidation reactions.

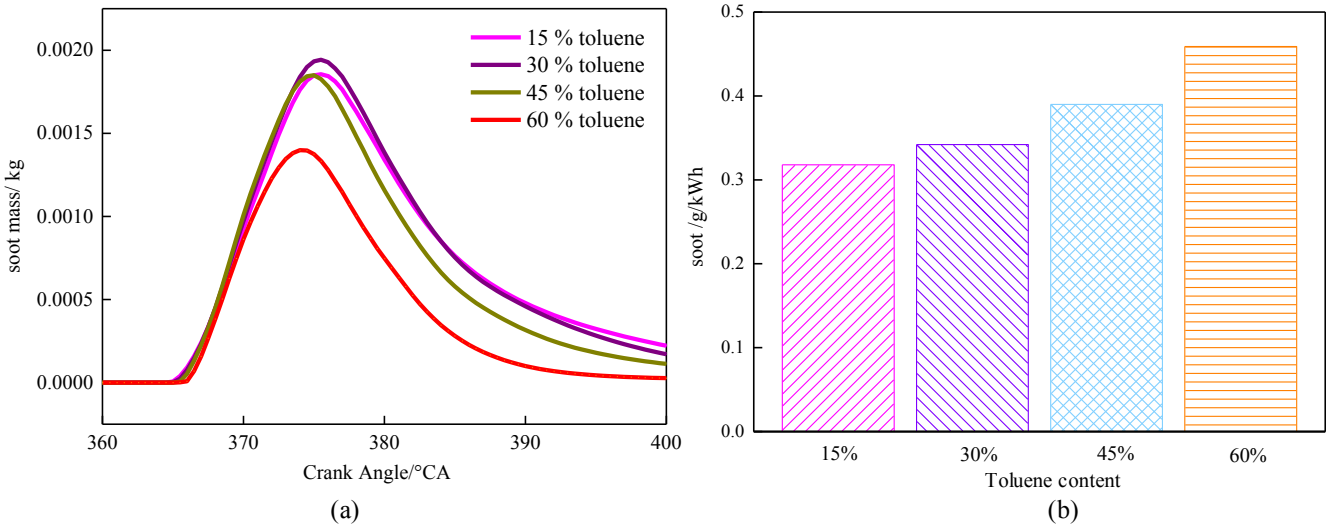

Fig. 7. Comparisons of soot for different toluene content: (a) soot mass variation with crank angle and (b) soot mass.

$$N + O_2 = NO + O \quad (1)$$

$$N + OH = NO + H \quad (2)$$

$$O + N_2 = NO + N \quad (3)$$

The quantity of N_2 and O_2 are same at the start of calculations for the different surrogate fuels models. The air-fuel ratio is large for the marine diesel engine due to the scavenging of two-stroke. So, the OH is important for the NO emissions. The large quantity of OH are produced by combustion reaction of toluene due to the reaction of $C_6H_5CH_2$ and HO_2. The calculated NO_x emissions increases when the toluene is used as one component of surrogate fuels.

Fig. 7(a) shows the variation of soot mass with the crank angle, and it can be seen that the soot mass reaches its maximum value. At the start of combustion, the soot oxidation rate is significantly lower than the soot formation rate, resulting in a drastic increase in soot mass. However, as the combustion progresses up to the maximum soot mass value, the soot oxidation rate overtakes the soot formation rate, resulting in decline of soot mass. It is worth noting that the variation trend of soot mass in Fig. 7(a) is not related to the toluene content of the surrogate fuels. Fig. 7(b) shows the variation of soot mass for different surrogate fuels, and it can be seen that the soot mass increases with increasing toluene content. Hiroyasu-NSC Model is used to simulate soot production. The sum of the hydrocarbon species is used as the soot formation species. The C_2H_2 is the important predecessor of soot formation [34]. The C_2H_2 is produced by the reaction:

$$C_6H_4O_2 + O = 2CO + C_2H_2 + CH_2CO \quad (4)$$

And, the $C_6H_4O_2$ is from the dehydrogenation oxidation of toluene. The toluene content has large influence on the soot mass.

Based on the simulation results, it is found that the surrogate fuel with 30% of toluene gives the best predictions for the NO_x emissions. The ratio of NO_x emissions is 0.97 for the surrogate fuel with 30% of toluene. In addition, there is good agreement in the in-cylinder pressure, effective power, and BSFC between simulations and experiments for this surrogate fuel. Hence, the surrogate fuel with 30% of toluene is determined to be the surrogate fuel to simulate the combustion process in a marine diesel engine based on the results.

4.3. Comparison of the in-cylinder pressures for surrogate fuels with different liquid properties

Previous studies have shown that different surrogate fuels have different liquid properties [35,36]. Fig. 8 shows the dynamic viscosity, surface tension, heat of evaporation and vapor pressure for *n*-tetradecane, toluene and diesel. These Data were obtained from the CONVERGE 2.3 software databank.

The dynamic viscosity and surface tension of diesel are higher than those of other fuels at high temperatures. Indeed, the dynamic viscosity of diesel is four times higher than that for toluene whereas the surface tension of diesel is higher than that for toluene by 30–50%. However, the vapor pressure and heat of evaporation of diesel are lower than those of other fuels. The physical properties of *n*-tetradecane are midway between the physical properties of diesel and toluene. However, the physical properties of *n*-tetradecane are similar to those for diesel. It is known that the differences in these physical properties will affect the fuel spray characteristics.

Commercial diesel fuels contain 30–35% of aromatics [19,37]. The effects of liquid fuels composed aromatic components on the performance of the marine diesel engine were also investigated in this study. The properties of toluene and *n*-tetradecane were applied in the parcel simulations. The effects of the physical properties of toluene can then be determined by comparing the results presented in Sections 4.1 and 4.2. The liquid properties and surrogate fuels can be found in Table 2.

Fig. 9 shows the simulation results of the in-cylinder pressures obtained for the surrogate fuels with different liquid properties. The longest ignition delay is observed for the surrogate fuel with 45% of toluene content. The ignition delay is decided by the mechanisms of surrogate fuels. The physical parameters of liquid have effect on the spray process. The lower values of surface tension leads to higher Weber numbers, resulting in slightly faster atomization. The higher vapor pressure curves for toluene results in higher evaporation rates. The homogeneity of mixture gas formation becomes better for the mixture with toluene. The effects of toluene physical parameters are smaller. However, the influence increases with toluene content. For the diesel-toluene mixture with 30% of toluene, the maximum in-cylinder pressure is higher than that obtained for the diesel–diesel mixture by 0.15 MPa. The physical properties of *n*-tetradecane makes the maximum in-cylinder pressure higher than others simulation results. Because the liquid parameters of *n*-tetradecane closer to the properties of toluene than those of diesel. For the *n*-tetradecane-toluene mixture with 30% of toluene, the maximum in-cylinder pressure is higher than that obtained for the diesel–diesel mixture by 0.53 MPa.

Fig. 10 shows the comparison of the indicated power and ISFC of the surrogate fuels with different liquid properties. It is evident that the liquid properties of toluene increase the indicated power for toluene content of liquid mixture less than 30%. The trends of indicated power has relationship with the changing of in-cylinder pressure. The

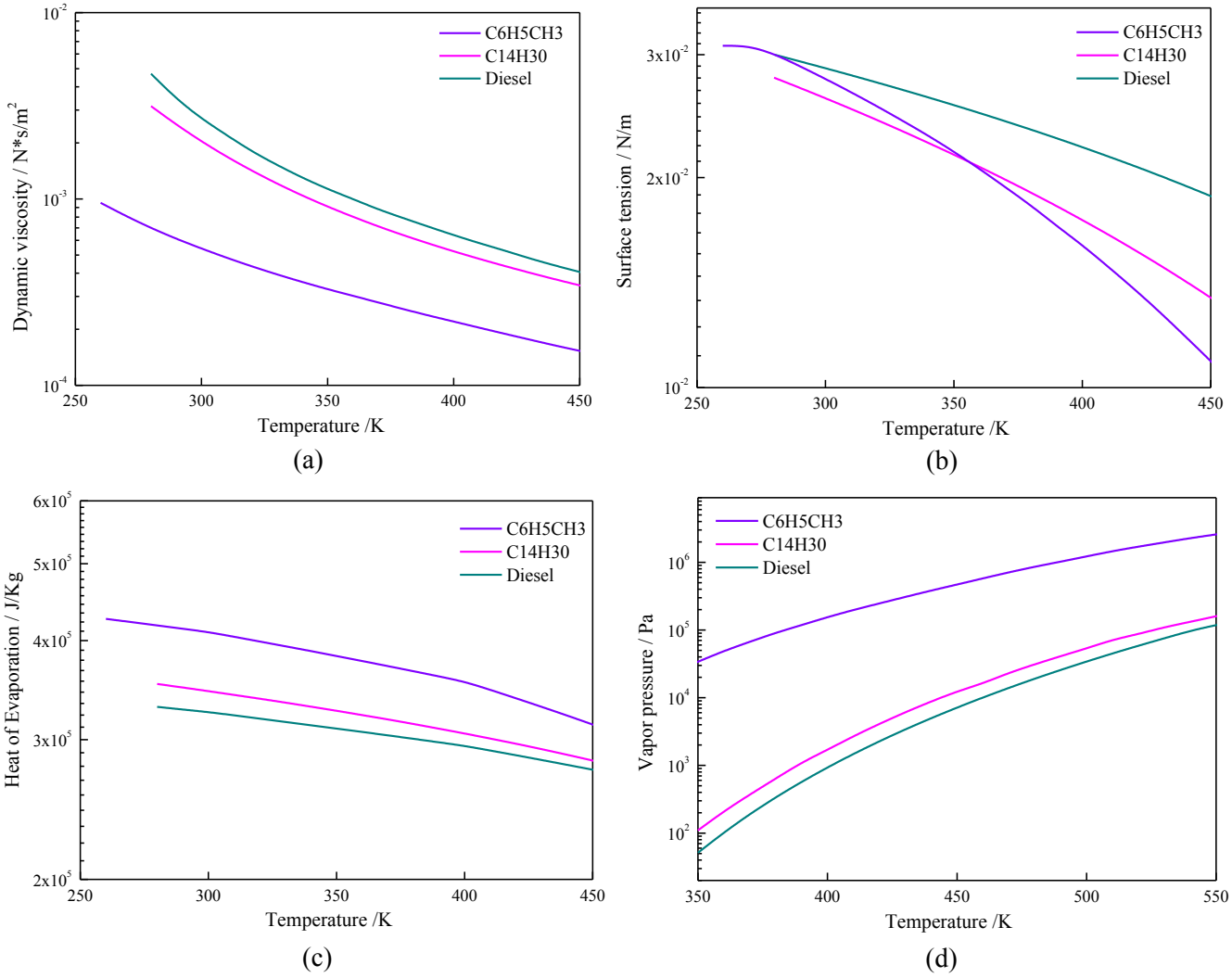

Fig. 8. Comparisons of liquid properties for *n*-tetradecane, diesel and toluene. (a) Dynamic viscosity, (b) surface tension, (c) heat of evaporation and (d) vapor pressure.

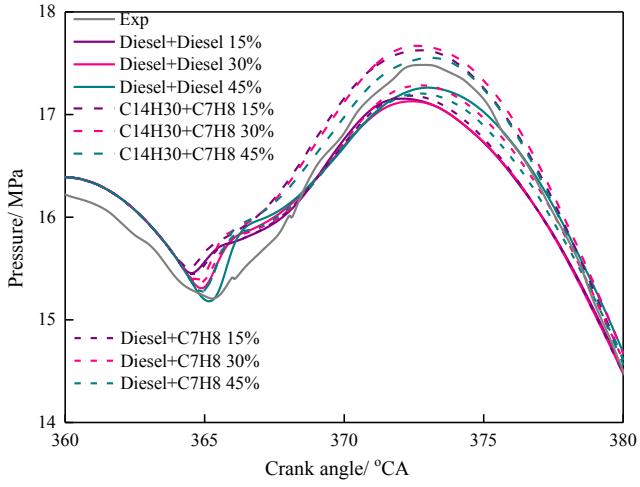

Fig. 9. Comparison of in-cylinder pressure for the surrogate fuels with different liquid properties.

indicated power of the toluene–diesel mixture is lower than the value for the diesel–diesel mixture with 15% of toluene by 7 kW. The indicated power of the toluene–diesel mixture is higher than the value for the diesel–diesel mixture with 30% of toluene by 12 kW. The effect of the physical properties of toluene decreases with an increase in the toluene content. The indicated power of the toluene–diesel mixture is lower than the value for the diesel–diesel mixture with 45% of toluene by 20 kW. The indicated power is lower than others results for the *n*-tetradecane-toluene mixture. A different trend is observed for the ISFC because the fuel injection mass flow rate is kept constant in the CFD simulations.

4.4. Comparison of the exhaust emissions for surrogate fuels with different liquid properties

The effects of surrogate fuels with different liquid properties on the NO_x emissions and soot were also investigated in this study. Fig. 11 shows the variations of NO_x emissions of the diesel–toluene, diesel–diesel, and diesel–*n*-tetradecane mixtures. The plotted values represent discrepancies between the simulation and experimental results. The physical properties of toluene increase the formation of NO_x emissions for mixtures with 30% of toluene. The faster atomization and higher evaporation rates of toluene make the mixture gas homogeneity during the ignition delay times. The fuel is burned completely, which makes the in-cylinder temperature increasing. However, the oxygen are also consumed. In general, higher in-cylinder temperature and fuels with higher oxygen content will lead to higher NO_x emissions. So, the

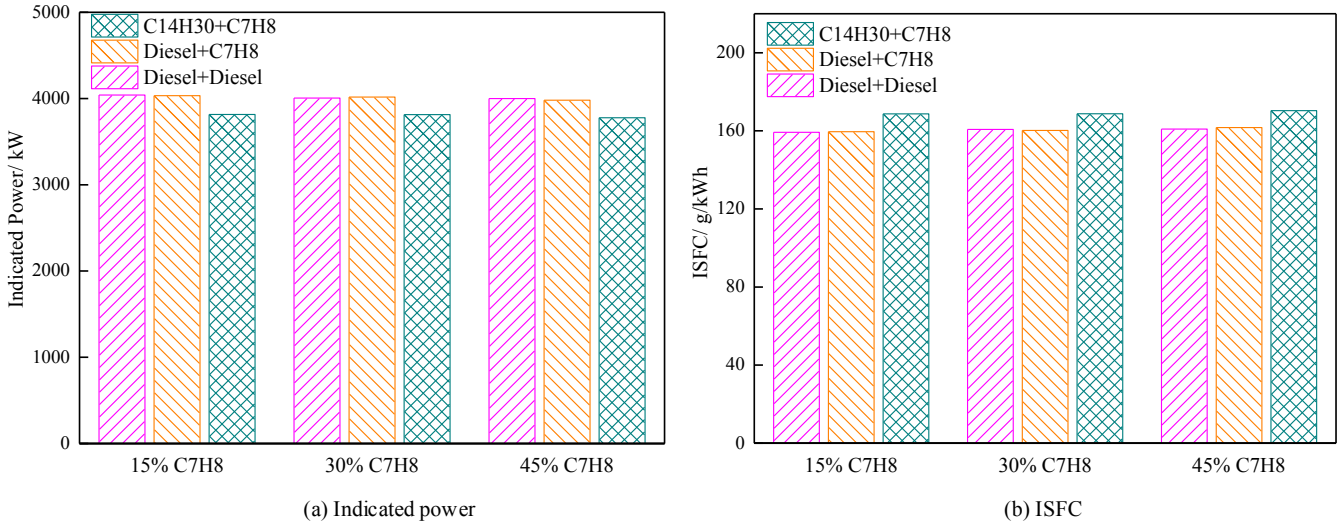

Fig. 10. Comparisons of indicted power and ISFC for the surrogate fuels with different liquid properties (a) indicted power and (b) ISFC.

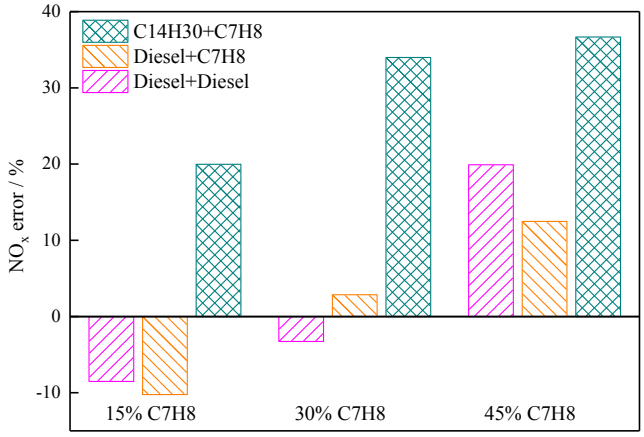

Fig. 11. Comparison of NO_x for the surrogate fuels with different liquid properties.

NO_x emissions have peak value with the increasing the toluene content in liquid fuels. The NO_x emissions of the toluene–diesel mixture are higher than the value for the diesel–diesel mixture with 30% of toluene by 0.77 g/kWh. However, the NO_x emissions of the toluene–diesel mixture are lower than the value for the diesel–diesel mixture with 45% of toluene by 0.94 g/kWh. However, the NO_x emissions are higher for the *n*-tetradecane-toluene mixtures compared with those for the diesel-diesel mixture.

Fig. 12 shows the in-cylinder temperature and equivalence ratio distributions for the diesel-diesel and diesel-toluene mixture with 30% of toluene. Indeed, the range where the in-cylinder temperatures are more than 2000 K is wider for the liquid fuel with toluene. The equivalence ratios are also higher when liquid fuels with toluene are used in the parcel simulations at the crank angle 365 °CA.

It is obvious seen that the errors of NO_x emission are large for the diesel–*n*-tetradecane mixtures compared with experimental data. The *n*-tetradecane is not used as physical properties of marine diesel fuel in parcel simulation. The error of NO_x emission is minimum for diesel-toluene mixture with 30% of toluene.

Fig. 13 shows the soot mass of the diesel–toluene, diesel–diesel, and diesel–*n*-tetradecane mixtures with different physical properties. It can be seen that physical properties of the liquid fuels with 30% of toluene only have a minor effect on the soot mass. The physical properties of *n*-tetradecane result in higher soot mass. The longer ignition delay of toluene improves fuel-air mixing and thus, more toluene is burned for fuel mixtures with higher toluene content, as shown in Fig. 12. The molecular structure of toluene includes a benzene ring, which promotes soot formation. However, toluene has longer ignition delay compared with that for *n*-tetradecane, which improves the combustion characteristics. Because the molecular structure and elemental composition of liquid fuels affect the combustion characteristics and exhaust emissions of marine diesel engines, it is important to choose the surrogate fuel to simulate the combustion process using CFD.

The ignition delay is an important parameter that can be used to assess the suitability of the surrogate fuel in simulating the combustion process in marine diesel engines. The ignition delay error can be determined by comparing the time at which the pressure at combustion start is observed between simulations and experiments. The in-cylinder pressure is related to the engine power and it is known that the surrogate fuel affects the in-cylinder pressure during the combustion process. Hence, the in-cylinder pressure is also an important parameter that can be used to evaluate the suitability of the surrogate fuel in emulating the combustion process of real fuels. The combustion of fuels (regardless whether the fuels are real fuels used in marine diesel engines or surrogate fuels) releases undesirable emissions to the environment and it is known that the regulations for NO_x emissions are more stringent compared with those for other exhaust emissions. For this reason, NO_x emissions can also be used to assess the suitability of the surrogate fuel for CFD simulations.

Fig. 14 shows the differences between the simulation and experimental results for the in-cylinder pressure and NO_x emissions and it can be seen that there is larger error for the NO_x emissions. Based on the results, it can be deduced that the liquid fuel with 30% of toluene is the most suitable surrogate fuel to simulate the combustion process of marine diesel engines since it has the lowest error for NO_x emissions (0.36) relative to that for the diesel–diesel mixture. There is good agreement in the maximum in-cylinder pressure between simulations and experiments during the combustion phase for the liquid fuel with 30% of toluene. The in-cylinder pressure errors at the start of combustion are 0.04 and 0.12 for the liquid fuel with 30% of toluene and diesel–diesel mixture, respectively, even though both fuels have the same ignition delay. In general, the surrogate fuel with 30% of toluene gives satisfactory results in simulating the combustion characteristics and exhaust emissions of the marine diesel engine, where the physicochemical properties of toluene are used in the parcel simulations.

5. Conclusion

In this study, numerical simulations were carried out using CFD

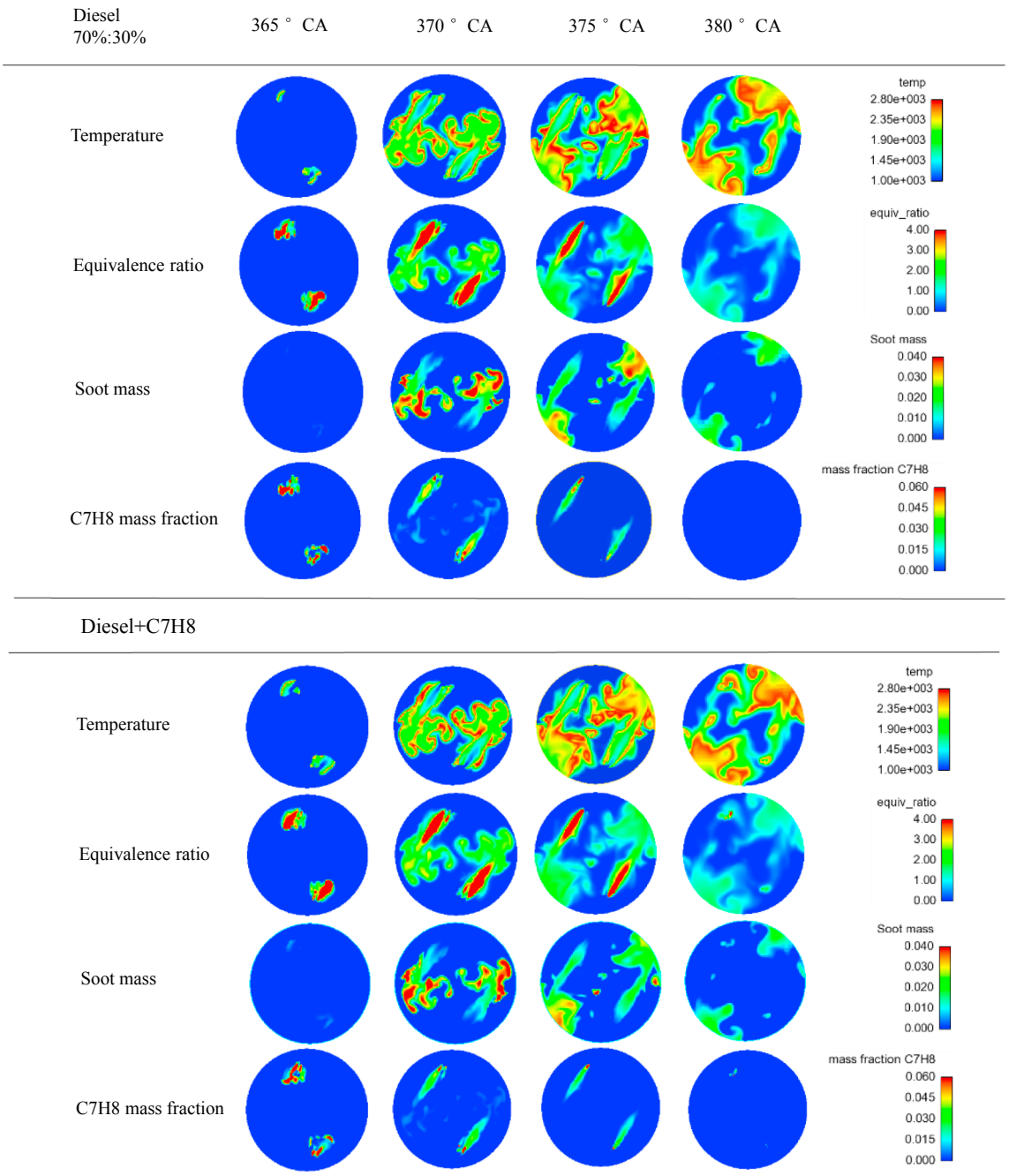

Fig. 12. Comparisons of in-cylinder temperature, equivalence ratio, soot mass and toluene mass fraction for the diesel-diesel and diesel-toluene mixture with 30% of toluene.

software to investigate the effect of toluene content in surrogate fuel on the combustion characteristics and exhaust emissions of a marine diesel engine. The liquid parameters were also researched to improve the accuracy of simulation model. The established simulation model was validated with the experimental data. The key findings of this study are presented as follows:

1. The ignition delay times increase with an increasing in toluene content of surrogate fuel. The power decreases with an increase in toluene content. However, the NO_x and soot mass are increase. The toluene content of multi-components surrogate fuel has directly effect on the simulation results, especially for the emissions.
2. It is not ignore that the influence of physical properties in liquid fuel on the performance of the marine engine. The nitrogen oxide show opposite tendency compared with the 45% and 30% of toluene content in the diesel-toluene mixture. The simulation results are higher when the diesel was replaced by the same content of *n*-tetradecane in liquid fuel.
3. The key parameters obtained from simulations were compared with those from experiments to show that the important of surrogate fuel and liquid properties. The *n*-tetradecane–toluene mixture with 30% of toluene was proposed as surrogate fuel of a marine diesel engine.

In general, the surrogate fuel proposed in this study is able to reduce errors in simulating the combustion process of a marine diesel engine. The results of this study indicate that the appropriate selection of surrogate fuel will enable scientists and engineers involved in combustion research to use chemical kinetics coupled with CFD simulations to

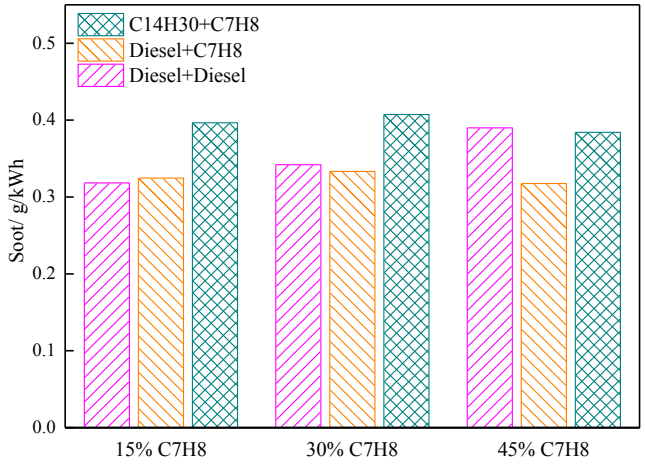

Fig. 13. Comparison of soot mass for the surrogate fuels with different liquid properties.

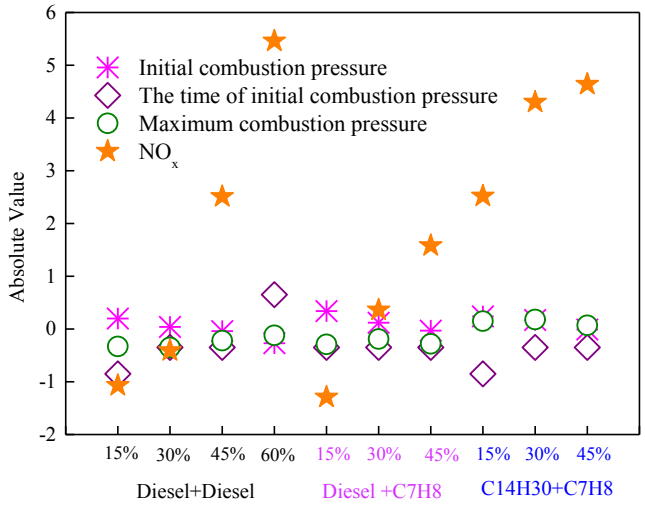

Fig. 14. Comparisons of key parameters for the simulation and experimental values.

simulate the combustion process in marine diesel engines with higher accuracy.

Acknowledgements

This work was supported by National Natural Science Foundation of China (No. 91641111 and No. 51806148) and Marine Low-Speed Engine Project (Phase I) of MIIT.

References

[1] Emission Standards (Internal: IMO Marine Engine Regulations). http://www.DieselNet.com/standards.
[2] S. Zhou, Y. Liu, J.X. Zhou, A study on exhaust gas emission control technology of marine diesel engine, Adv. Mater. Res. 864–867 (2013) 1804–1809.
[3] P. Geng, H. Mao, Y. Zhang, L. Wei, K. You, J. Ju, et al., Combustion characteristics and NOx emissions of a waste cooking oil biodiesel blend in a marine auxiliary diesel engine, Appl. Therm. Eng. 115 (2017) 947–954.
[4] L. Feng, J. Tian, W. Long, W. Gong, B. Du, D. Li, et al., Decreasing NOx of a low-speed two-stroke marine diesel engine by using in-cylinder emission control measures, Energies 9 (2016) 304.
[5] W. Ji, A. Li, X. Lu, Z. Huang, L. Zhu, Numerical study on NOx and ISFC co-optimization for a low-speed two-stroke engine via Miller cycle, EGR, intake air humidification, and injection strategy implementation, Appl. Therm. Eng. 153 (2019) 398–408.
[6] X. Jiang, H. Wei, L. Zhou, R. Chen, Numerical study on the effects of multiple-injection coupled with EGR on combustion and NOx emissions in a marine diesel engine, Energy Proc. 158 (2019) 4429–4434.
[7] S. Zhou, R. Gao, Y. Feng, Y. Zhu, Evaluation of Miller Cycle and fuel injection direction strategies for low NOx emission in marine two-stroke engine, Int. J. Hydrogen Energy 42 (31) (2017) 20351–20360.
[8] E. Sigurdsson, K.M. Ingvorsen, M.V. Jensen, S. Mayer, S. Matlok, J.H. Walther, Numerical analysis of the scavenge flow and convective heat transfer in large two-stroke marine diesel engines, Appl. Energy 123 (2014) 37–46.
[9] K. Zhang, Z. Liang, J. Wang, Z. Wang, Diesel diffusion flame simulation using reduced n-heptane oxidation mechanism, Appl. Energy 105 (2013) 223–228.
[10] C. Gong, M. Jangi, X.-S. Bai, Large eddy simulation of n -Dodecane spray combustion in a high pressure combustion vessel, Appl. Energy 136 (2014) 373–381.
[11] https://combustion.llnl.gov/.
[12] K.M. Pang, N. Karvounis, J.H. Walther, J. Schramm, Numerical investigation of soot formation and oxidation processes under large two-stroke marine diesel engine-like conditions using integrated CFD-chemical kinetics, Appl. Energy 169 (2016) 874–887.
[13] V. Stratsianis, P. Kontoulis, L. Kaiktsis, Effects of fuel post-injection on the performance and pollutant emissions of a large marine engine, J. Energy Eng. 142 (2016).
[14] K. Panagiotis, C. Christos, K. Lambros, Evaluation of pilot injections in a large two-stroke marine diesel engine, using CFD and T-φ mapping, in: The International Symposium on Diagnostics and Modeling of Combustion in Internal Combustion Engines, vol. 1, 2008.
[15] L. Maria, R. Juan, C. Laura, C. Luis, Effect of multiple injection strategies on emissions and performance in the Wärtsilä 6L 46 marine engine. A numerical approach, J. Clean. Prod. 206 (2019) 1–10.
[16] F. Perini, J.L. Brakora, R.D. Reitz, G. Cantore, Development of reduced and optimized reaction mechanisms based on genetic algorithms and element flux analysis, Combust. Flame 159 (2012) 103–119.
[17] V.R. Katta, S.K. Aggarwal, W.M. Roquemore, Evaluation of chemical-kinetics models for n-heptane combustion using a multi-dimensional CFD code, Fuel 93 (2012) 339–350.
[18] X. Sun, X. Liang, G. Shu, Y. Wang, Y. Wang, H. Yu, Development of a reduced n-tetradecane-PAH mechanism for application on two-stroke marine diesel engine, Energy Fuel (2016).
[19] Y. Zhang, M. Jia, P.F. Wang, Y.C. Chang, P. Yi, H. Liu, Z.X. He, Construction of a decoupling physical–chemical surrogate (DPCS) for practical diesel fuel, Appl. Therm. Eng. 149 (2019) 536–547.
[20] K. Anand, Y. Ra, R.D. Reitz, B. Bunting, Surrogate model development for fuels for advanced combustion engines, Energy Fuel 25 (2011) 1474–1484.
[21] W.J. Pitz, R. Seiser, J.W. Bozzelli, K. Seshadri, C.J. Chen, D. Costa, et al. Chemical kinetic study of toluene oxidation, in: 2gth International Symposium on Combustion, Sapporo, Japan, July 21–26, 2002.
[22] H. Barths, H. Pitsch, N. Peters, 3D simulation of DI diesel combustion and pollutant formation using a two-component reference fuel, Oil Gas Sci. Technol. 2 (1999) 233–244.
[23] J.C.G. Andrae, T. Brinck, G.T. Kalghatgi, HCCI experiments with toluene reference fuels modeled by a semidetailed chemical kinetic model, Combust. Flame 155 (2008) 696–712.
[24] T. Javed, C. Lee, M. AlAbbad, K. Djebbi, M. Beshir, J. Badra, et al., Ignition studies of n-heptane/iso-octane/toluene blends, Combust. Flame 171 (2016) 223–233.
[25] H. Wang, M. Yao, Z. Yue, M. Jia, R.D. Reitz, A reduced toluene reference fuel chemical kinetic mechanism for combustion and polycyclic-aromatic hydrocarbon predictions, Combust. Flame 162 (2015) 2390–2404.
[26] X. Liu, H. Wang, X. Wang, Z. Zheng, M. Yao, Experimental and modelling investigations of the diesel surrogate fuels in direct injection compression ignition combustion, Appl. Energy 189 (2017) 187–200.
[27] K. Zhang, Q. Xin, Z. Mu, Z. Niu, Z. Wang, Numerical simulation of diesel combustion based on n-heptane and toluene, Propul. Power Res. (2019) Available online 14 February.
[28] X. Sun, X. Liang, G. Shu, Y. Wang, Y. Wang, H. Yu, Effect of different combustion models and surrogate fuels on two-stroke marine diesel engine performance, Appl. Therm. Eng. 115 (2017) 597–606.
[29] P.J. O'Rourke, Collective Drop Effects on Vaporizing Liquid Sprays, Ph.D. thesis Princeton University, 1981.
[30] H.Q. Wei, X. Chen, G.F. Wang, L. Zhou, S.J. An, G.Q. Shu, Effect of swirl flow on spray and combustion characteristics with heavy fuel oil under two-stroke marine engine relevant conditions, Appl. Therm. Eng. 124 (2017) 302–314.
[31] http://www.idaj.cn.
[32] X. Sun, X. Liang, G. Shu, J. Lin, H. Wei, P. Zhou, Development of a surrogate fuel mechanism for application in two-stroke marine diesel engine, Energy 153 (2018) 56–64.
[33] H. Hiroyasu, T. Kadota, Models for combustion and formation of nitric oxide and soot in direct injection diesel engines, SAE Technical Paper, 760129, 1976.
[34] A. Jain, Y. Wang, W. Kulatilaka, Effect of H-atom concentration on soot formation in premixed ethylene/air flames, Proc. Combust. Inst. 37 (2) (2019) 1289–1296.
[35] C. Yang, Y. Kidoguchi, R. Kato, K. Miwa, Effects of fuel properties on combustion and emissions of a direct-injection diesel engine, Bull. M.E.S.J. 2 (2000).
[36] N. Kyriakides, C. Chryssakis, Lambros, Influence of Heavy Fuel Properties on Spray Atomization for Marine Diesel Engine Applications, 2009.
[37] W.J. Pitz, N.P. Cernansky, F.L. Dryer, F.N. Egolfopoulos, J.T. Farrell, D.G. Friend, et al., Development of an Experimental Database and Chemical Kinetic Models for Surrogate Gasoline Fuels. SAE.