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Research on the Soot Generation of Diesel Surrogate Mechanisms of Different Carbon Chain Length

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Abstract: This paper studies the generation process and emission characteristics of soot from Marine diesel engine. On the basis of Particulate size mimic (PSM) detailed soot model, the parameters related to soot generation obtained from the reaction mechanism calculation of 3 surrogate of different carbon chain length: n-heptane, n-tetradecane and n-tetradecane-toluene were compared and analyzed including precursor of soot, quality and density of soot, particle size distribution of empirical soot model. The results show that the soot nucleation stage of n-tetradecane-toluene mechanism was slightly more consistent than that of n-tetradecane mechanism with the experimental results, far more consistent than that of n-heptane mechanism. The intensity of surface growth and aggregation stage is greater, which is reflected in the soot precursor: acetylene and A4, and leads to that the soot produced by the mechanism of n-tetradecane and n-tetradecane-toluene is small in quality but large in quantity. The particle size distribution calculated by n-tetradecane and n-tetradecane-toluene mechanism is closer to the experimental data than that calculated by n-heptane mechanism. Then combustion process of n-tetradecane and n-tetradecane-toluene mechanism is more suitable for marine engine, which is reflected in the higher temperature and the smaller equivalent ratio in the cylinder.

Keywords: marine diesel engine; soot; numerical simulation; soot model; surrogate fuels reaction mechanism

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1. Introduction

With the increase demand of trade and transportation in recent years, The particulate emissions of transportation have caused more and more serious pollution [1]. Therefore, it is very important to study and control the emission of pollutants from ships. However, the large size and power of Marine diesel engine will cost a lot of manpower and material resources to carry out the physical experiment on it, so the simulation study on its particulate emissions is very beneficial.

The generation of soot is an extremely complicated process in which a lot of physical and chemical changes occur [2]. Although many details of the formation process of soot are still controversial in academic circles, there is a preliminary consensus on the general process of its formation: The initial formation of soot requires a certain precursor (chemical reaction between molecules in the gas phase) [3]. Nuclear reactions occur between macromolecules to form soot particles (the initial formation of soot particles). The surface growth process of particles became true by the adsorption of gas phase molecules on the surface of particles and the condensation process of soot particles is came true by the collision reaction between soot particles (surface growth and condensation of soot particles). The oxidation of precursor and soot particles will reduce the amount of soot [4].

In terms of the research on the soot generation process of diesel: Glassman proposed that acetylene is an important precursor of soot by diesel combustion, which was later confirmed by Richter and Howard [5,6]. Due to the fact that some intermediate components cannot be generated by acetylene in the process of soot formation, the reaction conditions are limited, and the experimental verification is extremely complicated, so polycyclic aromatic hydrocarbons (PAHs) are more likely to be the precursor of soot formation [7]. The production of precursor depends on the change of combustion reaction mechanism. The earliest research is to replace diesel with something similar.

Among them, the cetane number of n-heptane is close to that of diesel, and among many of the mechanisms of n-heptane, study of Curren et al. is the most classic including 544 components and 2446 reactions of n-heptane reaction mechanism [8]. Later generations use sensitivity analysis method, direct diagram method and quasi steady state analysis to simplify the reaction mechanism of n-heptane. Wanhua Su and Haozhong Huang [9] proposed a new reduced called 'SKLE model' chemical kinetic model containing 40 species and 62 reactions for the Homogeneous Charge Compression Ignition (HCCI) combustion of n-Heptane. This model was able to describe the two-stage HCCI combustion in an engine reasonably, but the result of ignition delay time has a large error in low equivalence ratio. Now the simplified mechanism can control the reaction group scores and number within 100 [10,11].

The physical properties of n-tetradecane are similar to that of diesel oil, so n-tetradecane is an ideal substitute for diesel oil. Struckmeier et al. [12]. studied the effects of properties of fuel components on the ignition and combustion properties of the fuel blend using tetradecane to solve the chemical reaction equations. Panagiotis et al. [13]. use computational fluid dynamics (CFD) and T-4 mapping to study the effects of advanced injection strategies on the performance of marine diesel engines using tetradecane as a surrogate fuel. It was demonstrated that, at an appropriate timing, fuel savings of the order of 1.7% could be achieved by adding a pilot injection, without increasing NOx emissions. Raptotasios et al. [14] investigated the NOx reduction potential of two-stroke marine diesel engines with EGR using the n-tetradecane as surrogate fuel in the calculated model, and results showed that the NOx emission could be reduced to the value of the Tier III requirement, when the rate of EGR was increased to 35% for the 4T50ME-X test engine.

However, with the deepening of the research, we need to develop a multi-component mixed alternative to the combustion reaction mechanism, for that PAHs is an important precursor of soot nucleation, and diesel contains aromatic components, which are mostly simple ring structure, so the alkyl benzene toluene is considered to be added to the multi-component alternative to the combustion mechanism as the simplest. At present, a large number of studies have explored the reaction path of toluene itself, then explored the reaction mechanism of multi-component mixture mixed with toluene, and carried out relevant experimental verification, which has made considerable progress in the research on the reaction mechanism of toluene [15–20]. Ra et al. [21] developed multi-component fuels mechanism for an internal combustion engine including oxidation and reduction mechanisms of n-tetradecane, toluene, cyclohexane, dimethyl ether, ethanol, and methyl butanoate. The final version of the mechanism consisted of 113 species and 487 reactions, and this present multi-component combustion model provided reliable performance for combustion prediction. Wei et al. [22] studied the physical properties of soot from n-heptane–toluene and n-heptane combustion. Soot produced by n-heptane-toluene combustion usually shows more primary particles than n-heptane soot. Therefore, toluene was used to obtain a better prediction mechanism for PAHs and soot.

In a word, the development trend of diesel surrogate combustion mechanism is from single component to multi-component, from detailed mechanism to simplified mechanism. The objective of the development of substitute combustion mechanism is to simplify the mechanism as much as possible and obtain higher computational efficiency on the basis of guaranteeing the superior performance of simulated combustion. In addition, it is important to explore the carbon chain length of surrogate that better match diesel. This paper study the parameters related to soot generation obtained from the reaction mechanism calculation of 3 surrogate of different carbon chain length: n-heptane, n-tetradecane and n-tetradecane-toluene.

2. Simulation Model

2.1. n-Heptane Mechanism

As mentioned above, n-heptane has been proven by numerous studies to be a classic fuel substitute for simulating diesel ignition combustion processes. The n-heptane mechanism selected in this paper is the simplified mechanism of n-heptane constructed by Liu et al. [23]. (This is referred to as n-heptane mechanism).

The mechanism of n-heptane is combined with PAHs reaction mechanism to adapt to soot generation simulation preferably. In addition, the original mechanism of oxidation reaction of n-heptane mainly includes the following three mechanisms:

Low temperature mechanism: it comes from the small detail reaction mechanism optimized by Juan c. Perance [24]. On the basis of 40 reaction components and 235 step elemental reactions of SD, 8 step elemental reactions were eliminated, and 4 reaction components and other 14 step elemental reactions were added. The final oxidation mechanism at low temperature mainly includes the following reactions:

$$\mathrm{C_7H_{16} + O_2 \Leftrightarrow C_7H_{15} + HO_2}$$

$$\mathrm{C_7H_{16} + X \Leftrightarrow C_7H_{15} + XH}$$

$$\mathrm{C_7H_{15} + O_2 \Leftrightarrow C_7H_{15}OO}$$

$$\mathrm{C_7H_{15}OO \Leftrightarrow C_7H_{14}OOH}$$

$$\mathrm{C_7H_{14}OOH + O_2 \Leftrightarrow OOC_7H_{14}OOH}$$

The final optimization mechanism could well match the characteristics of ignition delay in the low-temperature combustion area of n-heptane [24].

High temperature mechanism [9]: it comes from the high temperature part of SKLE mechanism that Su and Huang et al. connected on the basis of Griffiths mechanism. The important reaction at high temperature includes two parts, one is the formation of a large number of free radicals, the other is the dissociation of H_2O_2. As follows:

$$\mathrm{H + O_2 \Leftrightarrow O + OH}$$

$$\mathrm{H_2O_2 \Leftrightarrow OH + OH}$$

PAH mechanism: PAH mechanism is proposed by Wang et al. [25]. The polycyclic aromatic hydrocarbon formation and oxidation reaction of the PAH mechanism mainly through the following path of one to four benzene rings (A1 to A4): A1 → INDENE (C9H8) → A2 → A2R5 → A3 → A4.

Liu et al. removed the duplicate part of the three-part mechanism and simplified it using the sensitivity analysis method on the basis of the three-part combination mechanism. Finally, the 78-step elemental reaction and 57 reaction components was obtained, which is suitable for the n-heptane reaction mechanism of soot generation simulation. The original mechanism of its main oxidation reaction is shown in the Figure 1:

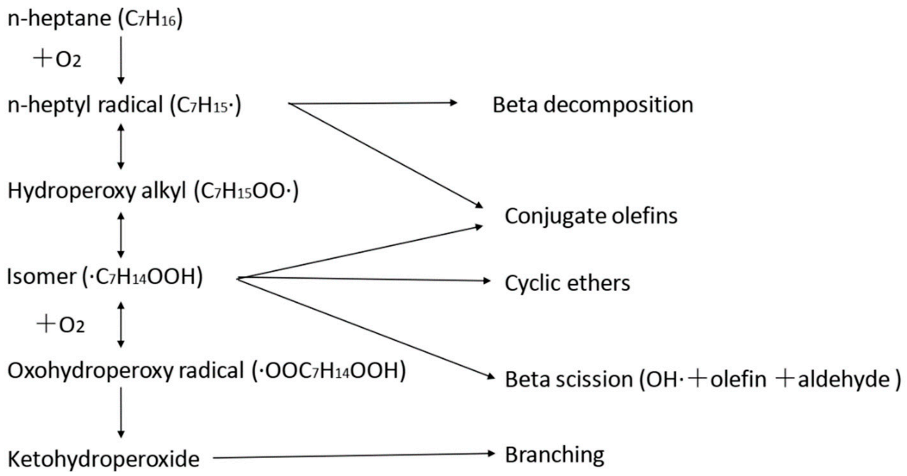

Figure 1. Oxidation mechanism of n-heptane [20].

The mechanism has passed the verification of ignition delay time and other parameters, which can be used for further simulation research.

2.2. n-Tetradecane Mechanism

As mentioned above, the physical parameters of n-tetradecane are closer to real diesel, so it is also a common diesel surrogate [13]. The mechanism of n-tetradecane is selected to simulate the generation of soot in low-speed two-stroke Marine diesel engines. The selected mechanism of n-tetradecane was derived from the simplified mechanism of n-tetradecane from our previous study [26]. (This is referred to as n-tetradecane mechanism).

This mechanism of n-tetradecane was constructed based on the "semi-decoupling" method proposed by Liu et al. [27]: the alkane combustion can be divided into two categories: one is primarily a small molecular components of the reaction mechanism, mainly through which describe the flame propagation and reaction, and the reaction process has little relationship with the type of alkanes. The other is to describe the ignition characteristics of fuels by coupling small molecule mechanism, which is applicable to various fuels. Sun et al. applied this mechanism construction method and select the elementary reactions involving small molecules such as H2 and CO by Klippenstein et al. [27,28]. The C2–C3 chemical reaction mechanism of small molecule reaction overreacting to low temperature is derived from the gri-3.0 reaction mechanism which is relatively mature at present. The low-temperature reaction of n-tetradecane was mainly based on the research results of Chang et al. [29] and constructed a semi-detailed reaction mechanism of n-tetradecane containing 74 reaction components and 341 steps. After that, Sun et al. simplified the semi-detailed mechanism of n-tetradecane using the direct diagram method in chemkin-workbench software, verified and adjusted the error, and finally obtained the simplified mechanism of n-tetradecane for 62 reaction components and 279 step elemental reactions. The original mechanism of its main oxidation reaction is shown in the Figure 2:

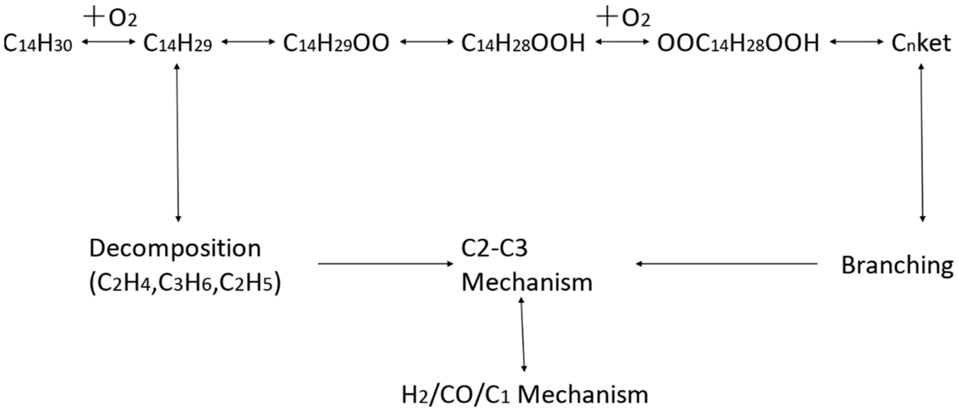

Figure 2. Oxidation mechanism of n-tetradecane.

This mechanism has passed the verification of ignition delay time and other characteristics, which can be used for further research.

2.3. n-Tetradecane-Toluene Mechanism

As mentioned above, the current research trend is to develop the reaction mechanism of multi-component combustion substitutes, so as to simulate the reaction changes of each component in diesel during combustion preferably. Diesel oil contains a large number of aromatic hydrocarbon compounds in addition to the alkanes described above. Therefore, it is necessary to use the reaction mechanism of multi-component diesel substitutes containing aromatic compounds to simulate the generation of soot in low-speed two-stroke Marine diesel engines. As the simplest aromatic compounds—toluene, is the first choice to study aromatic compounds, according to its oxidation reaction path as we can see in Figure 3, toluene reaction will have the production of acetylene, which is generated soot or important precursor chemicals. In this paper, two-component reaction mechanism of n-tetradecane and toluene constructed by Sun et al. [30] was adopted for subsequent studies.

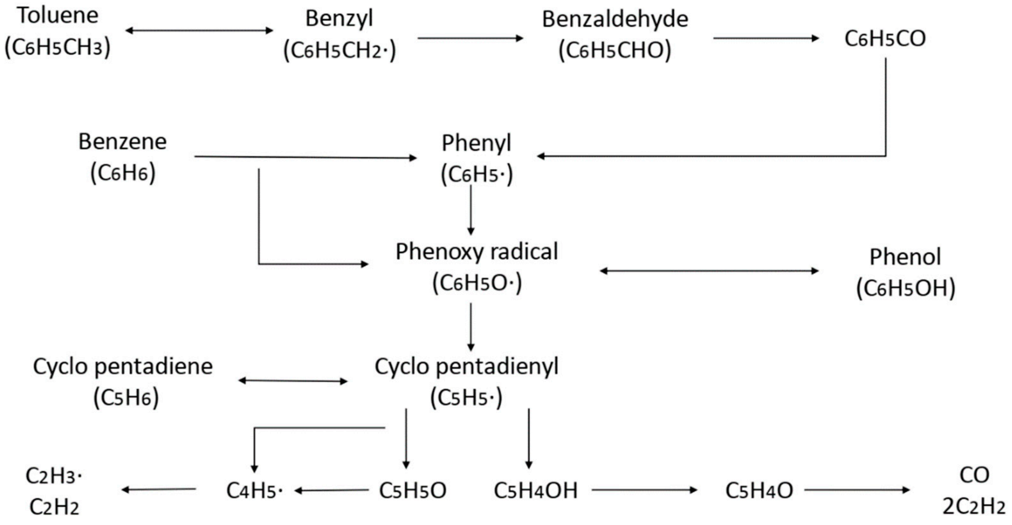

Figure 3. Main reaction of oxidation of toluene.

This mechanism also adopts the "semi-decoupling" method and adds the toluene reaction mechanism that has been verified on the basis of the combustion mechanism of the basic substitute for the framework mechanism of n-tetradecane that has been constructed [26]. In the CHEMKIN-Workbench software, two reaction mechanisms were combined and n-tetradecane was used as the unit reaction, then finally build the reaction mechanism of n-tetradecane-toluene, which included 85 reaction components and 317 steps of unit reaction. Similarly, the mechanism has passed the verification of ignition delay time and other characteristics, and the reaction mechanism of the diesel substitute can be used for the subsequent simulation study of soot generation of low-speed two-stroke Marine diesel engines.

2.4. Preliminary Basic Model

The object in this paper is the main engine of a low-speed two-stroke large ship whose model is 6S35ME-B9. The detailed parameters and indexes of this model under 100% working conditions are shown in Table 1. The geometric 3D CFD model structure diagram of 6S35ME-B9 engine which is constructed using the geometric structure parameters of 6S35ME-B9 engine is shown in Figure 4, include one cylinder with a part of scavenge box and exhaust port.

Table 1. Parameters of 6S35ME-B9.

Parameter Name	Parameter Value
cylinder diameter (mm)	350
stroke (mm)	1550
number of cylinders	6
displacement (L)	159
length of connecting rod (mm)	1550
Rated speed (r/min)	142
Rated power (kWh)	3575

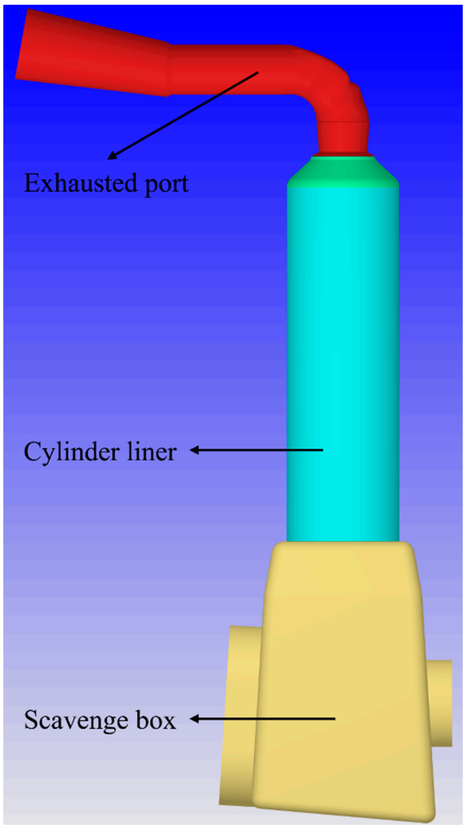

Figure 4. The 3-D geometric structure of marine diesel engine.

In addition, it is also necessary to set the relevant calculation parameter model of the engine as shown in Table 2, and calibrate the 3d numerical simulation model based on the experimental data of 6S35ME-B9 engine under 100% load conditions using the calculation model combined with the n-tetradecane simplified model of Chang et al. [29].

Table 3 shows the difference between experimental data and machine model calculation. In general, in the calculation, the cylinder pressure and fuel consumption error less than 5% is acceptable. It can be seen that the maximum error is the output power, which is 1.99% within the acceptable range.

Table 2. Simulation models.

Name	Model
Spray crushing model	KH-RT
Turbulence model	RNG k-ε
Combustion model	SAGE
Droplet evaporation model	Frossling
Droplet collision model	NTC
Turbulent droplet diffusion model	O'Rourke
Droplet impact model	Wall Film

Table 3. The comparison of pressure between experiment data and simulated data.

	Experimental Value	Simulation Value	Error (%)
Maximum compression pressure (bar)	162.47	163.96	0.92
Maximum combustion pressure (bar)	174.83	173.92	−0.52
Outbreak of moment (°CA)	365.35	364.4	0.26
Output power (kW)	3575	3646.02	1.99
Effective fuel consumption (g/kWh)	180	176.54	−1.92

In the previous work, it has been obtained that the detailed model in the soot model is closer to the experimental value, so the soot model will use PSM. This paper will study the influence of the fuel surrogate mechanism including n-heptane mechanism, n-tetradecane mechanism and n-tetradecane-toluene mechanism in the category of gas phase reaction dynamics on the soot simulation. Since most ships in the emission control area use LFO (light fuel oil), the mechanism of this paper mainly focuses on light diesel.

3. Results and Discussion

This section will analyze the similarities and differences of several surrogate in the generation of soot from precursor of soot, combustion parameters, and empirical model to generate hiroy-soot, quality and density of soot, particle size distribution of soot particles, then make evaluation.

3.1. Precursor Substances

The generation of soot is closely related to many intermediate products in the combustion process, among which acetylene is an important reaction source for Hydrogen abstraction acetylene addition (HACA) and the generation of PAHs, and the precursor of PSM model selected in this paper is also PAHs. [31] Therefore, this section will explore the effects of different diesel surrogate combustion mechanisms on the generation of acetylene and A4 which represents PAHs.

(1) Influence on the formation of acetylene:

Figure 5 shows the trend of the mass of acetylene calculated by three mechanisms. The trend of acetylene generation calculated by n-tetradecane and n-tetradecane-toluene mechanism is almost the same, which changes continuously and the mass of acetylene generation reaches its peak at the most violent moment of combustion reaction. After that, the mass of acetylene generation gradually decreases with the end of combustion process, and finally maintains at the order of 10^{-8} kg. However, there is a difference in quantity: the acetylene of n-tetradecane—toluene is more than that of n-tetradecane. The mass of acetylene obtained using n-heptane mechanism is in constant fluctuation, and its mass is far less than that of the other two mechanisms. Eventually, it will stabilize at the order of 10^{-15} kg, which is also far less than that of the other two mechanisms.

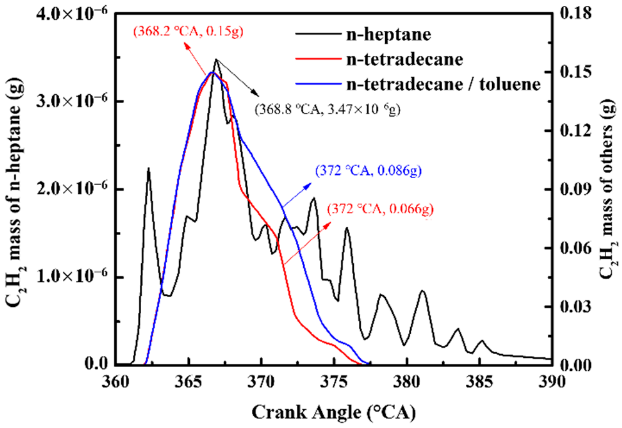

Figure 5. Generation mass of C2H2 for different combustion mechanisms.

Figure 6 shows the mass distribution of acetylene in cylinder of three mechanisms. The mass distribution obtained by n-heptane mechanism is significantly smaller than that of the other two mechanisms, and compared with the other two mechanisms, it takes longer to stabilize (n-heptane mechanisms is not stable after 385 °CA, n-tetradecane and n-tetradecane toluene mechanism has been stable at 380 °CA). The mechanism of n-tetradecane and n-tetradecane-toluene has little difference either in the tendency of acetylene mass generation or the distribution in cylinder.

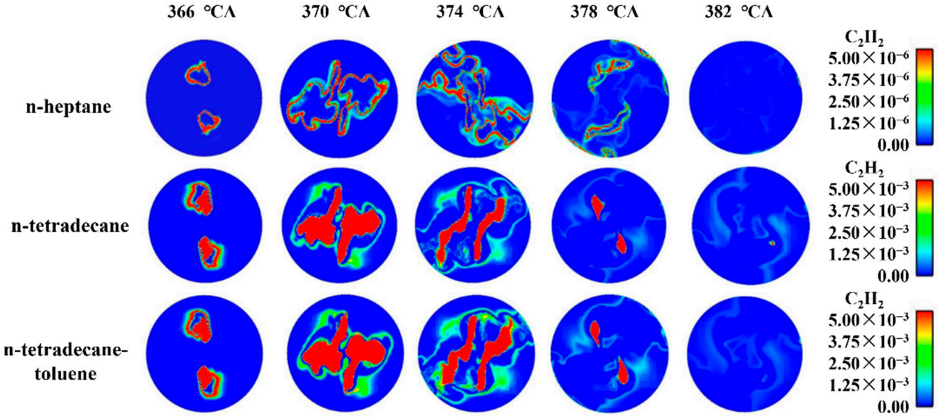

Figure 6. Mass distribution of C2H2 in the cylinder of different combustion mechanisms.

Figures 7 and 8 are, respectively, the path diagram analysis of acetylene generation in n-heptane and n-tetradecane. The n-tetradecane has more pathways to form acetylene, and that each pathway has fewer steps. In the same time period, about 8% C of n-heptane was converted to acetylene, 28% C of n-tetradecane was converted to acetylene, and conversion rate of toluene is 69% as we can see from Figure 9. Obviously, the acetylene production of n-tetradecane and toluene is much higher than that of n-heptane. Since toluene only accounts for 15% of n-tetradecane-toluene, it is slightly more than pure tetradecane.

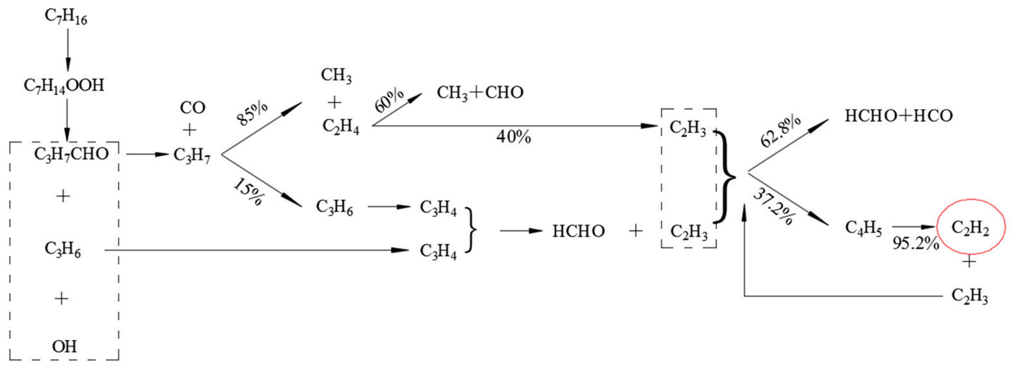

Figure 7. Acetylene formation path in n-heptane.

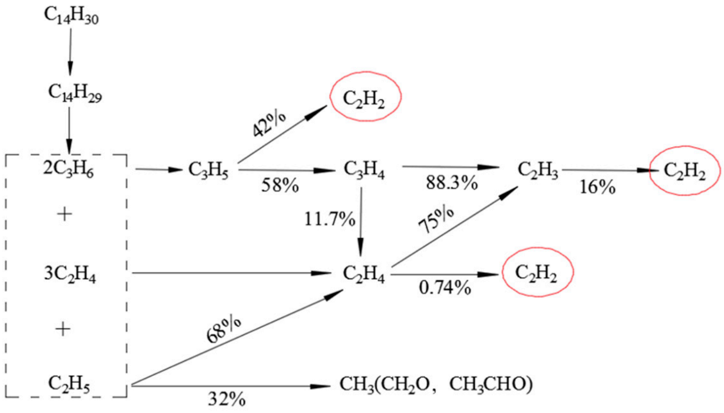

Figure 8. Acetylene formation path in n-tetradecane.

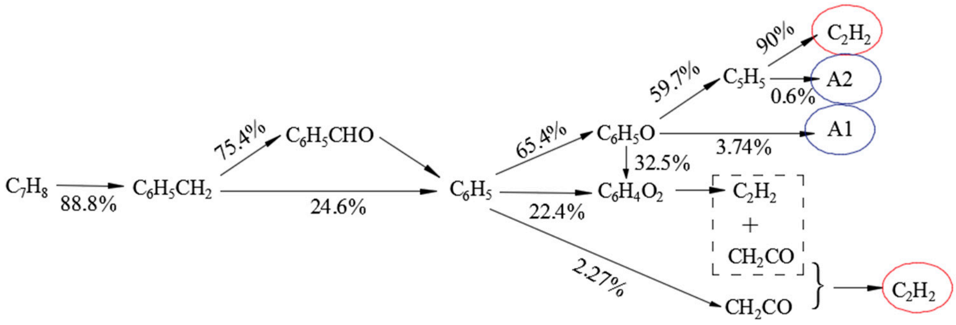

Figure 9. The formation path of acetylene and aromatic hydrocarbons in toluene.

And acetylene is an important substance of soot surface growth (HACA mechanism), so the surface growth process of n-heptane is relatively slow.

(2) Influence on the generation of PAHs

In the detailed soot—PSM model used in this study, PAHs is an important precursor of soot generation, and A4 is most important in PAHs. A large number of studies have shown that A4 can be used as the initial nucleating material [32–34]. Therefore, this study selected A4 as the research object to explore the influence of different combustion mechanisms on precursor substances in the process of soot formation.

Figure 10 shows the tendency of A4 mass generated using three diesel alternative fuel mechanisms. As can be seen from the figure, A4 calculated by n-heptane rose to a maximum value, and fluctuated slightly at the peak value, then decreased slowly. However, the mass of A4 generated by n-tetradecane and n-tetradecane-toluene mechanism first reached a peak value, and declined rapidly, then the rate of decline slowed down, after that the rate of decline began to accelerate, and finally stabilized with the end of combustion. In addition, in terms of specific values, the mass of A4 obtained using n-tetradecane-toluene mechanism is slightly larger than that of n-tetradecane mechanism and much larger than that of n-heptane mechanism.

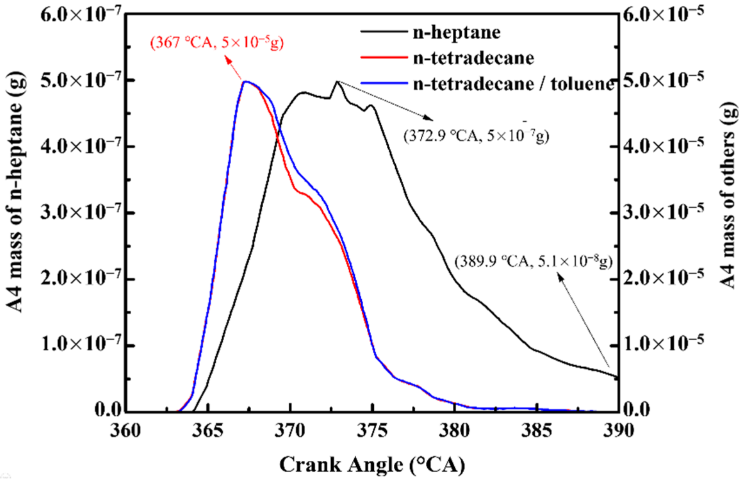

Figure 10. Generation mass of A4 for different combustion mechanisms.

Figure 11 shows the mass distribution in A4 cylinder calculated by the mechanism of three diesel substitutes. Obviously, the mass of A4 obtained by n-heptane mechanism is significantly lower than that of n-tetradecane and n-tetradecane-toluene mechanism. The mass distribution map obtained using n-tetradecane mechanism and n-tetradecane-toluene mechanism is similar. Moreover, the region where A4 generated is similar to acetylene, further confirming the theory that acetylene is an important source of A4 generation. Compared with the other two mechanisms, the A4 mass produced by n-heptane mechanisms takes longer to stabilization (n-heptane mechanisms is stable at 385 °CA, n-tetradecane and n-tetradecane-toluene mechanism has been stable at 380 °CA).

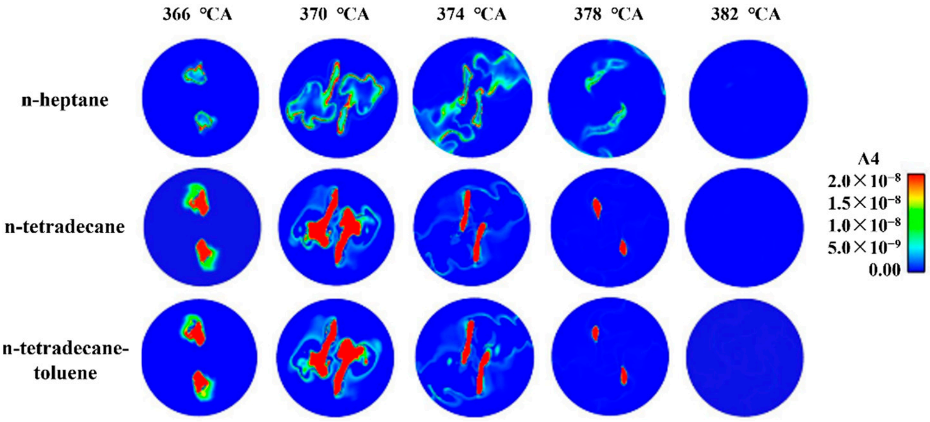

Figure 11. Mass distribution of A4 in the cylinder of different combustion mechanisms.

Figures 12 and 13 show the A4 generation of n-heptane and n-tetradecane, respectively. As we can be seen, the A4 production path of n-tetradecane is more than that of n-heptane. Moreover, the A4 of n-heptane is mostly grown on the basis of A1, while the A4 of n-tetradecane is not only grown on the basis of A1, but also has aggregation process of polycyclic aromatic hydrocarbon, so n-tetradecane produces more A4 than n-heptane. For n-tetradecane-toluene, we can see from Figure 9 that toluene can supply the first ring A1 required, and due to its proportion, A4 production of n-tetradecane-toluene slightly more than n-tetradecane.

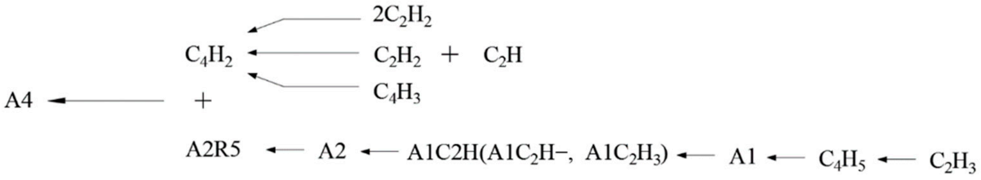

Figure 12. A4 formation path in n-heptane.

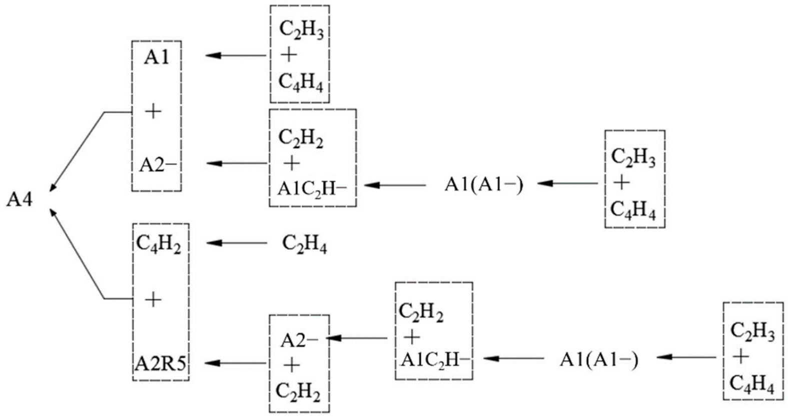

Figure 13. A4 formation path in n-tetradecane.

As mentioned above, A4 is the initial nucleating material, so it can be seen from the above results that the nucleation stage of n-tetradecane and n-tetradecane is more intense, while that of n-tetradecane-toluene is slightly more intense than that of n-tetradecane.

3.2. Comparison of Combustion Parameters

As the combustion mechanism of diesel surrogate is closely related to the combustion process, different diesel surrogate process parameters are firstly compared [35]. The generation and evolution of soot are closely related to the temperature and equivalent ratio in the cylinder of diesel engine. Therefore, the temperature distribution and equivalent ratio distribution are selected as the combustion parameters.

(1) equivalent ratio distribution:

Figure 14 shows the coupling of n-heptane mechanism, n-tetradecane mechanism and n-tetradecane-toluene mechanism with PSM detailed soot model to simulate the in-cylinder combustion and soot generation of low-speed two-stroke Marine diesel engine, and the calculated in-cylinder equivalent ratio of the distribution diagram. The distribution form of in-cylinder equivalent ratio of each mechanism is similar, all of them are especially large at the initial stage near the nozzle, and then tend to average as the fuel spreads and burns. However, there are differences in the distribution of equivalent ratio for each mechanism: in the corresponding inner cylinder area, the equivalent ratio of n-heptane mechanism at each moment after combustion is higher than that of n-tetradecane and n-tetradecane-toluene mechanism. When comparing the mechanism of n-tetradecane and n-tetradecane-toluene, they are almost the same in terms of the distribution of equivalent ratio and magnitude, and only have slight differences.

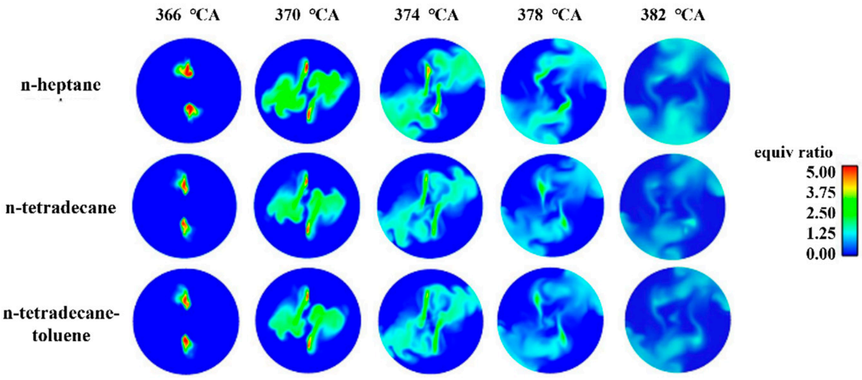

Figure 14. Equivalent ratio distribution of different combustion mechanisms.

(2) temperature distribution

Figure 15 shows the temperature distribution in cylinder with different combustion mechanisms. After injecting oil at a 362.6 °CA, the temperature in the cylinder of n-tetradecane and n-tetradecane-toluene mechanism was significantly higher than that of n-heptane mechanism in the whole spray combustion process, and the phenomenon was similar in the subsequent combustion process. As mentioned above, the equivalent of n-heptane is higher than that of n-tetradecane and n-tetradecane-toluene at each combustion moment, which indicates that the combustion reaction rate of n-heptane mechanism is slower than that of the other two mechanisms, so the temperature of n-heptane mechanism is lower. Cylinder temperature of both n-tetradecane and n-tetradecane-toluene is similar, only after the crankshaft Angle of 374 °CA there will be a slight difference near the injector nozzle.

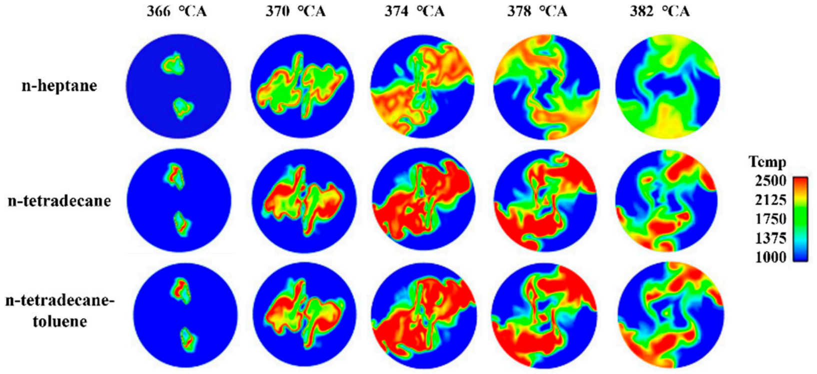

Figure 15. In-cylinder temperature distribution of different combustion mechanisms.

3.3. Empirical Soot Model

In this section, the quality and in-cylinder distribution of soot calculated using Hiroy-NSC empirical soot model when three different diesel substitutes are used for combustion mechanism are mainly compared.

(1) variation trend of hiroy-soot

Figure 16 is the variation curve of hiroy-soot quality generated by three different combustion mechanisms. All the three hiroy-soot quality generation curves are generated rapidly and form a sharp peak after the combustion starts, then decrease rapidly, and finally slowly increase to a certain value. Moreover, it can also be seen from the figure that the calculated hiroy-soot quality of n-heptane mechanism is much higher than that of the other two mechanisms at the peak value. At the crankshaft angle of 477 °CA, namely the time when the exhaust valve is open, the hiroy-soot quality of n-heptane is also significantly higher than that of the other two mechanisms. However, there is no obvious difference between n-tetradecane and n-tetradecane-toluene.

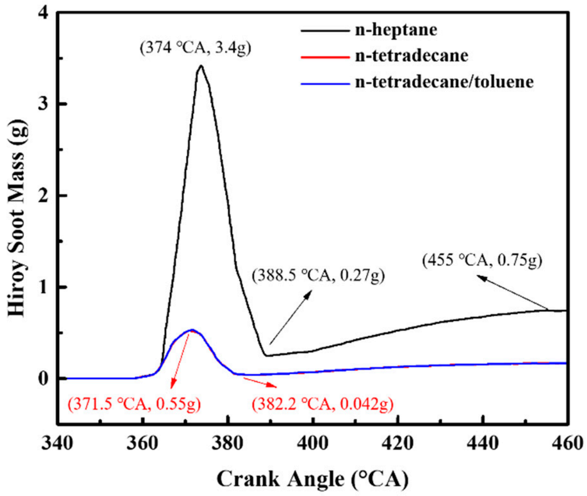

Figure 16. Generation mass of Hiroy-Soot for different combustion mechanisms.

(2) Hiroy-Soot distribution

Figure 17 shows the internal mass distribution of hiroy-soot generated by three different substitution mechanisms in cylinder. The inner mass distribution area as well as the hiroy-soot mass generated by n-heptane mechanism is significantly higher than that of other two mechanisms. By comparing with the temperature and equivalent ratio distribution mentioned above, it can be found that the in-cylinder region where hiroy-soot is generated is also the region with high in-cylinder temperature and equivalent, which verifies the theory that soot is generally generated in the in-cylinder region with high temperature and high equivalent ratio. Moreover, due to low temperature in n-heptane mechanism and high equivalent ratio, combustion is not fully achieved, then the hiroy-soot quality produced by it is higher. By comparing the two mechanisms of n-tetradecane and n-tetradecane toluene, the calculated hiroy-soot quality difference is very small, and only produces a little difference at the nozzle of the injector, which can be ignored. It is also caused by the fact that the two obtained in the previous text are similar in temperature and equivalent ratio distribution.

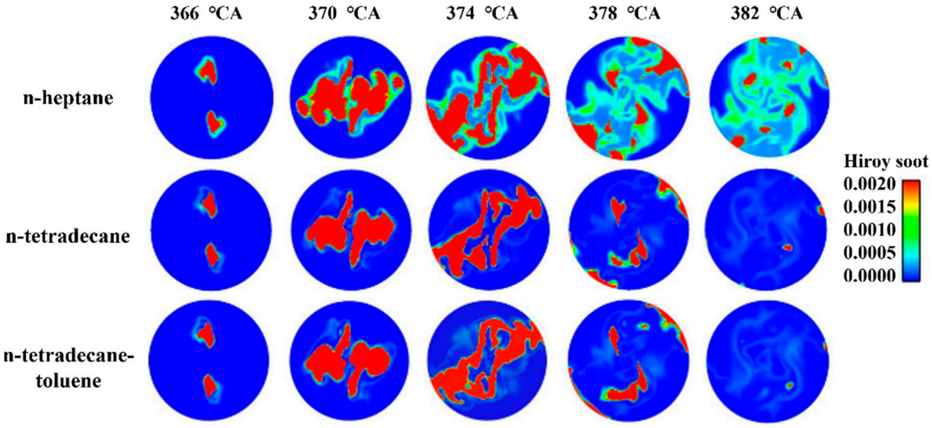

Figure 17. In-cylinder mass distribution of Hiroy-Soot with different combustion mechanisms.

3.4. Soot Mass and Quantity Density

The most important index of soot generation is the quantity density and mass of soot. Therefore, this section compares the quantity density and mass of soot obtained by three diesel substitutes.

(1) Mass of soot

Figure 18 shows the mass tendency of soot generated in the cylinder. The mass of soot produced by n-heptane rises at the beginning of combustion, then decreases slowly, and gradually stabilizes at the end of combustion. The mass tendency of soot formation in the mechanism of n-tetradecane and n-tetradecane-toluene is almost the same. In both cases, the mass of soot is generated in large quantities after the combustion starts, and rapidly reduced by oxidation. Finally, at the end of combustion, the mass of soot formation tends to be stable. In terms of specific values, the mass of soot obtained using n-tetradecane mechanism at the peak was slightly lower than that obtained by n-tetradecane-toluene mechanism, but in the subsequent combustion process until the moment when exhaust valve was opened at 477 °CA, the mass of soot obtained by n-tetradecane and n-tetradecane-toluene mechanism is almost the same. However, the mass of the soot calculated by n-heptane was lower than that of the other two at the peak, but the gap gradually narrowed as the combustion progressed due to the rapid oxidation of the other two mechanisms. The n-heptane mechanism has about half that of the other two mechanisms when the exhaust valve is open.

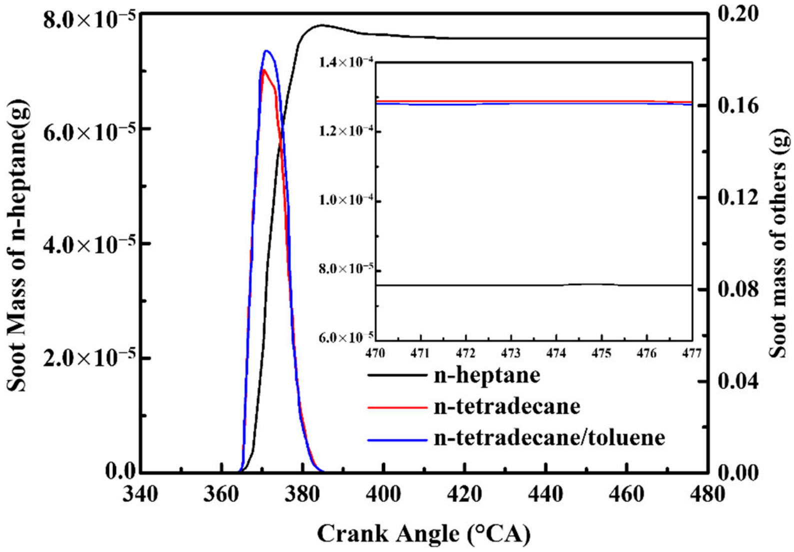

Figure 18. In-cylinder soot mass generation curve of different combustion mechanisms.

(2) quantity density of soot

Figure 19 shows the tendency of quantity density of soot calculated using three diesel replacement mechanisms. Similarly, n-tetradecane mechanism and n-tetradecane-toluene mechanism had the same trend of soot quantity density generation, but the tendency of n-heptane was different. Moreover, at the peak of combustion, the soot density of n-heptane is much lower than that of the other two mechanisms. When exhaust valve is opened at 477 °CA, the density of soot obtained using n-heptane mechanism is about 28 times as high as that of the other two mechanisms.

The amount of soot produced by n-heptane is larger than that of n-tetradecane and n-tetradecane-toluene, but the quality is much smaller than that of the latter two, which can be verified by the results obtained from the date of precursor in this paper: Since the acetylene produced by n-heptane is far less than the latter two, the surface growth and aggregation process are relatively slow. The smaller the amount of accumulated soot particles, the larger the number of them, and the smaller the mass of soot particles. Moreover, the amounts of A4 produced by the latter two is even larger than that of n-heptane, so the mass of n-heptane particles will be even lower.

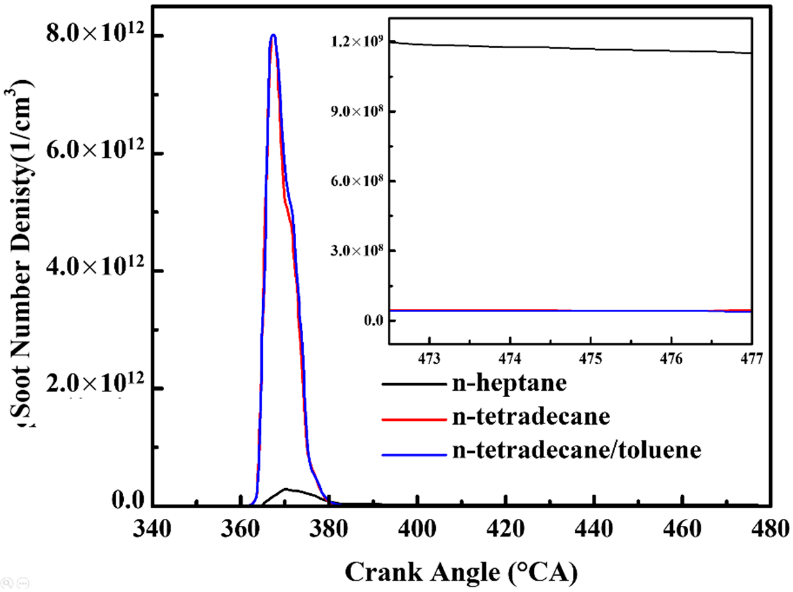

Figure 19. Formation curve of in-cylinder soot number density in different soot models.

3.5. Particle Size of Soot Particles

Since this study using PSM model in detail, where we can analyze the particle size of soot, but can only acquire the information of the soot size distribution from 0–100 nm in CONVERGE.

Figure 20 shows the distribution of mass fraction and particle size changes of soot calculated using different combustion mechanisms: most of the soot calculated using n-heptane mechanism is concentrated in 5~20 nm, and particles with larger particle size almost do not exist. However, the particle size of soot emitted by low-speed two-stroke Marine diesel engines is mostly over 100 nm. It can be seen from the figure that the particle size distribution tendency calculated by n-tetradecane and n-tetradecane-toluene mechanism is almost the same, and the particle size is mostly over 100 nm.

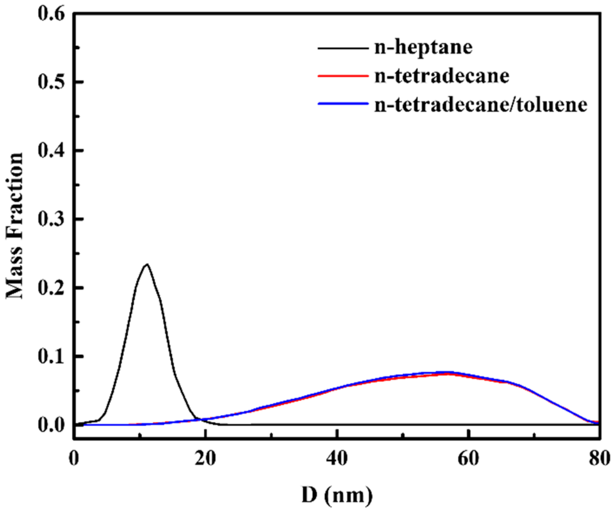

Figure 20. Particle size distribution of soot with different combustion mechanisms.

4. Conclusions

In this paper, three different mechanisms of diesel oil substitution were studied, namely n-heptane mechanism, n-tetradecane mechanism and n-tetradecane-toluene mechanism. The combustion parameters, precursor generated, mass and quantity density of generated soot calculated using the three mechanisms were, respectively, compared, and the following conclusions were obtained:

(1) The temperature obtained by n-tetradecane and n-tetradecane-toluene mechanism was higher than that by n-heptane mechanism. The equivalent ratio is lower than that of n-heptane. Proving that the combustion process of first two mechanisms is more intense than that of n-heptane.

(2) Hiroy-soot is mainly generated in the inner cylinder area with high equivalent ratio. Since the equivalent ratio calculated by n-heptane mechanism is higher, the Hiroy-soot mass calculated by n-heptane mechanism is larger than that of the other two mechanisms. However, the data of soot generation obtained by this empirical model is not acceptable due to its inconsistency with the actual situation.

(3) The mass of A4 obtained using the mechanism of n-tetradecane-toluene was slightly larger than that of n-tetradecane and much larger than that of n-heptane. Namely, the initial nucleation stage of n-tetradecane-toluene and n-tetradecane mechanism was relatively intense.

(4) The mass of acetylene calculated using n-tetradecane-toluene mechanism is slightly larger than that of n-tetradecane mechanism and much larger than that of n-heptane mechanism. Compared with the nucleation stage of soot, the surface growth and aggregation stage of n-tetradecane-toluene and n-tetradecane mechanism were more intense than that of n-heptane mechanism.

(5) Due to the nucleation stage of n-tetradecane-toluene and n-tetradecane mechanism is more intense, while the surface growth and aggregation stage is even more intense, which leads to the result that the soot is large in mass but small in quantity.

(6) Since the diesel used in marine engines has more macromolecular components, the mechanism developed for conventional diesel oil is not suitable for marine engine simulation. In the future, soot model suitable for marine engine should be developed to obtain more accurate emission results in the simulation process of marine engine performance test.

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