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Study on the Emission Characteristics in Renewable Energy Combustion under Different Working Conditions of Marine Two-Stroke Diesel Engine

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Abstract. In this paper, MAN 6S35ME-B9 two-stroke diesel engine is taken as the research object. By constructing a detailed combustion reaction mechanism including CH_4, $C_4H_{10}O$, nitrides and other substances, CHEMKIN-PRO is used to simulate the same fuel mixing ratio and excess air coefficient. Under the condition of 1.5, the temperature, NO mole fraction and NH_3 mole fraction in the reactor change and study the factors affecting the pollutant emission of marine diesel engine with the crank angle under different working conditions. The simulation shows that with the decrease of diesel engine speed, the maximum temperature of combustion reaction and the temperature at exhaust opening are obviously reduced. At the same time, mole fraction of NO and NH_3 decreases with the decrease of rotational speed, and there is no nitride production in the combustion reaction at 25%.

1.Introduction

Renewable energy refers to a kind of energy that can be continuously used and recycled in nature. [1] With the emergence of the world oil energy crisis, the importance of renewable energy is realized by the people. [2] During the "14th Five-Year Plan" period, renewable energy accounted for more than 50% of the increase in primary energy consumption.[3] Biofuels are receiving increasing public and scientific attention, driven by factors such as uncertainties related to oil price, green-house gas emission, and the need for increased energy security and diversity.[4-6] Bioalcohol fuel is a renewable energy, more in line with the future direction of energy development, from the whole ecological cycle[7] , the use of biological methods to produce alcohol fuel can be near zero CO_2 emissions.[8] Butanol is a very competitive renewable biofuel for use in internal combustion engines given its many advantages.[9] The compatibility of butanol with diesel is good, so there is no need to make major changes to the existing engine structure, and you can use butanol fuel with a concentration of almost 100%.[10] The purpose of research is to study n-butanol and LNG emission of nitride during combustion according to reaction mechanism. It is the basic research to reduce nitride emissions because of MARPOL VI Tier III regulations on NO_x emissions.

2.Technical parameters of diesel engine

Low speed two stroke diesel engine MAN 6S35ME-B9 was used to carry out the experiment in this study. The main parameters of MAN 6S35ME-B9 diesel engine are rated power of 3570 KW, the rated speed of 142 $r\cdot min^{-1}$, compression ratio of 21 , cylinder diameter of 350 mm , stroke of 1550 mm , sweep port timing of -38/38 (°)CA , exhaust valve timing of -64/98 (°)CA . In this study, the homogeneous charge compression ignition reactor in the software of CHEMKIN-PRO was used as reactor model. Comparing with the compression ratio of ordinary gasoline engine, HCCI engine is higher, the purpose is to improve combustion efficiency. According to parameters of the diesel engine, the 100% load condition of the reactor is set to the rated speed of 142 r/min, 129 r/min at 75% load, 112.8 r/min at 50% load and 89.5 r/min at 25% load.

3.Reaction mechanism and chemical reaction kinetics model

The combustion of the mixed fuel is simulated by CHEMKIN-PRO software. The reaction is required at different rotation speeds of the reactor when the mixing ratio of $C_4H_{10}O$ and CH_4 was 4:6. The reaction mechanism in the simulation comes from the reaction mechanism of the software itself, including the detailed kinetic and thermodynamic data of the reactants, products and intermediates. The model includes both thermodynamic and kinetic information required for the combustion stage of the mixed fuel, and also includes the three elements of C, H and O required for the study. In the combustion reaction stage of the mixed fuel, N, H and O elements will react to produce NH_x and NO_x. Reaction mechanism of $C_4H_{10}O$ containing nitrogen oxides reaction mechanism to simulates the combustion reaction production of NO_x and NH_x.

Base on the chemical reaction equation, the equation

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of $C_4H_{10}O$ and CH_4 in complete combustion is:

$$C_4H_{10}O+6O_2 \rightarrow 4CO_2+5H_2O \quad (1)$$

$$CH_4+2O_2 \rightarrow CO_2+2H_2O \quad (2)$$

When the excess air coefficient that meets the combustion conditions is 1.5 and the fuel mixing ratio is constant, according to Formulas (1) and (2), The ratio of O and N and the molar mass required for complete combustion of the fuel mixture at four speeds can be obtained. Argon is an inert gas. It does not react with other substances at room temperature and does not dissolve in liquid metal at high temperature. In this paper, argon is added to ensure that the molar fraction of reactants is the same at different rotational speeds, which ensures the uniqueness of the reaction variables. As shown in Table 1, the mole mass of air and argon required for combustion under different working conditions when the mixing ratio of $C_4H_{10}O$ and CH_4 is 4:6.

Table 1. The quality of mixed fuel and air under different conditions

Serial number	1	2	3	4
Working condition (%)	100	75	50	25
Revolution speed (r/min)	142	129	112.8	89.5
N-butyl alcohol (mol)	6.04	4.53	3.02	1.51
CH4 (mol)	0.87	0.65	0.44	0.22
Oxygen (mol)	18.12	13.59	9.06	4.53
Nitrogen (mol)	76.92	57.69	38.46	19.23
Argon gas (mol)	3.05	28.54	54.03	79.51

4.Result and analysis

HCCI is a widely concerned combustion mode. Like traditional gasoline engines, the reactants injected into the cylinder and the required air are very uniform, but its ignition mode in the same way as a diesel engine, and the combustion results are achieved by piston compression combustion of mixed gases.

Fig 1 shows that the in-cylinder temperature of $C_4H_{10}O$ and CH_4 burning at four speeds. In Fig 1, with increase of crank angle, the temperature increases slowly at first, when the crank angle increases sharply at 0°, The temperature in the cylinder rises rapidly until it reaches the maximum temperature, and then the increase of crank angle decreases slowly until the exhaust port opening. Explain the reasons for the above phenomena: due to the upward movement of the piston, the mixed gas is compressed to increase pressure in the reactor, consequence of a slow increase in temperature ; explain the reason why the temperature rises abruptly at 0°: the temperature rises to a certain value with the piston moves to 0°, and the mixed fuel in the cylinder is compressed and ignited, at the same time, a lot of heat is releassed, resulting in a sudden increase in the temperature in the reactor. Because the combustion process is more rapid, the piston is pushed downward, and the temperature in the reactor decreases slowly. It can be seen from the simulation results that as the speed of the diesel engine continues to decline, the maximum temperature in the cylinder and the exhaust temperature gradually decreases. When the speed is 89.5 r/min, the maximum temperature in the cylinder is 1690.97 K, it is 2038.92 K at 112.8 r/min, it is 2234.87 K at 129 r/min and it is 2364.55 K at 142 r/min. the temperature of exhaust port opening is 430.07 K at 89.5 r/min, it is 652.93 K at 112.8 r/min and it is 865.51 K at 129 r/min, it is 1040.562 K at 142 r/min. Compared with 142 r/min, the maximum temperature of the reactor at 129 r/min decreased by 5.48%, and the exhaust temperature decreased by 16.82%. At 112.8 r/min, the maximum temperature decreased by 13.77%, and the exhaust temperature decreased by 37.25%. At 89.5 r/min, the maximum temperature decreases by 28.49%, and the exhaust temperature decreases by 58.67%. That is, in the case of the same amount of fuel, reducing the speed of the diesel engine can effectively reduce the maximum temperature in the cylinder and the exhaust temperature.

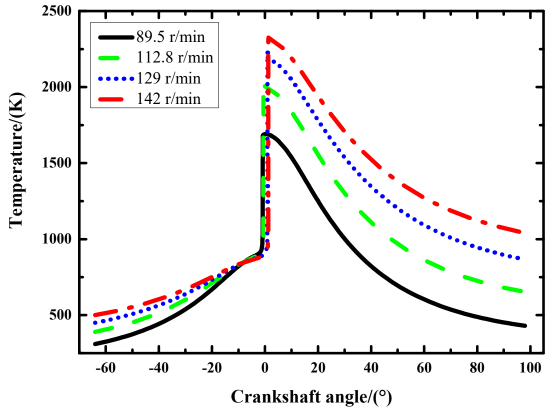

Fig 1. In-cylinder temperature of mixed fuel combustion at different speeds

Fig 2 shows the relationship between crank angle and molar fraction of NO produced by the combustion of mixed fuel at different speeds. When the angle of the crankshaft angle increases to 0°, the fluctuation of mole fraction of NO in the reactor is relatively small, which explains the phenomenon that there is no obvious change: the mixed fuel does not react and does not produce NO in the reactor. When the crank angle increases to 0°, the mixed fuel is compressed because of the temperature reaching 2000K. The N_2 and O_2 undergo a massive oxidation reaction, resulting in a sharp increase in NO mole fraction. Then, with the increase of crank angle, mole fraction of NO decreases rapidly. When the crank angle increases to about 20°, The molar fraction of NO showed a slow downward trend until the exhaust port opening. The decreasing trend of NO mole fraction was explained: The reaction equation of NO participation is analysed. As shown in Fig 3, corresponding reaction equation and main reaction equation of NO participation when the rotation speed is 129 r/min and the ratio of CH4 to C4H10O is 4:6 and the crank angle is 5.66°. As shown in Fig 3 NO plays not only the role of reactants, but also the role of combustion products according to the listed reaction equations. These include $NH_2+NO \Leftrightarrow NNH+OH$, $HNO+H \Leftrightarrow NO+H_2$, $NH+NO \Leftrightarrow N_2O+H$ and $N+OH \Leftrightarrow NO+H$, NO is the reactant.

$NO+H(+M) \Leftrightarrow HNO(+M)$, $NH_2+NO \Leftrightarrow N_2+H_2O$, NO is a combustion product. Calculated based on the above data, the decrease of NO mole fraction is due to the formation of NNH, N_2O, N, HNO.

It can also be seen from Figure 2 that when the reactor speed is 89.5 r/min, the mixed fuel combustion does not produce NO, and as the speed increases, the molar fraction of NO generated by combustion gradually increases. As shown in Fig 4 the change of NO molar fraction when the exhaust port is opened at different rotational speeds. From the diagram, it can be concluded that the NO molar fraction is 1.32×10^{-7} when the exhaust port opening at 142 r / min, and the NO molar fraction is 5.33×10^{-8} when the exhaust port is opened at 129 r/min, which decreases by 40.37%. When the exhaust port opening at 112.8 r/min, the molar fraction of NO is 1.93×10^{-8}, and the molar fraction decreases by 14.62%. With the increase of reactor speed, the molar fraction of NO generated by the reaction gradually increases.

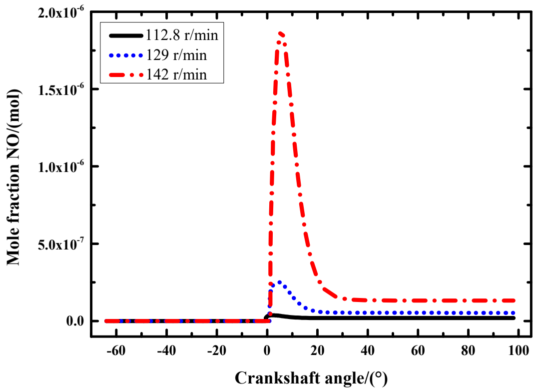

Fig 2. Mole fraction of NO produced by the combustion of mixed fuel at different speeds

with the decrease of rotation speed, the phenomenon that molar fraction of NO decreases is explained: the lower rotation speed of the reactor, the lower temperature during reaction process, and then the shorter the oxidation reaction time of N_2 and O_2, as the result of the less the production of NO. When the rotational speed is 89.5 r/min, the maximum temperature of the reaction is too low, so NO is not formed.

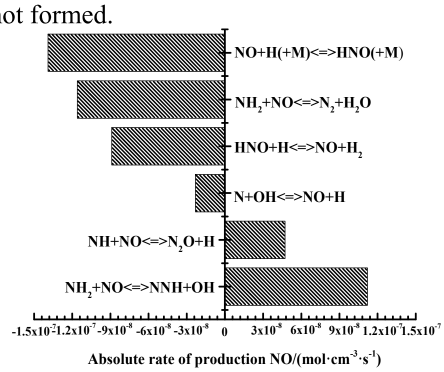

Fig 3. Main reaction equations involved in NO and the yield of the corresponding reaction equations.

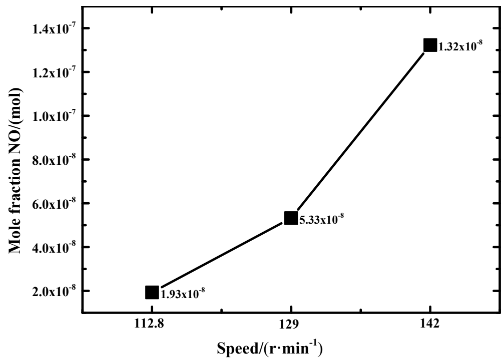

Fig 4. Mole fraction of NO when the exhaust port is opened at different speeds

As shown in Fig 5, the relationship between the crank angle and molar fraction of NH_3 in the two-stroke low-speed HCCI reactor of mix fuels at four different speeds. According to the Fig 5, with the increase of crank angle, the initial mole fraction of NH_3 did not undulate. When the crankshaft angle is closed to 0°, mole fraction of NH_3 increased sharply in the reactor . As the piston moves down, the molar fraction of NH_3 increases slowly before exhaust port opening. The increasing trend of the molar fraction of NH_3 was explained, and the reaction equation of NH_3 participation is analyzed. the efficiency of the main reaction equations involving NH_3 is shown in Fig 6. At the same time, the corresponding reaction equations in the rotation process are listed. speed is 129 r/min, the ratio of CH4 to C4H10O is 4: 6, and the crank angle is 5.66°. From the reaction equations listed, NH_3 plays not only the role of reactants, but also the role of combustion products in the combustion process. In chemical reactions $NH_3+OH \Leftrightarrow NH_2+H_2O$, NH_3 is the reactant. And in the chemical reaction $NH_3+H \Leftrightarrow NH_2+H_2$ and $NH_3+M \Leftrightarrow NH_2+H+M$ NH_3 is the product. Calculated based on the above data, the mainly due to the increase of NH_3 mole fraction is that part of NH_2 reacts to form NH_3. Fig 5 shows the change of NH_3 molar fraction when the exhaust port is opened at different rotational speeds. It can be seen in Fig 5 that the molar fraction of NH_3 is 1.32×10^{-7} when the exhaust port is opened at 142 r/min, and the molar fraction of NH_3 is 5.33×10^{-8} when the exhaust port is opened at 129 r/min, which decreases by 40.37%. When the exhaust port was opened at 112.8 r/min, the molar fraction of NH_3 was 1.93×10^{-8}, and the molar fraction decreased by 14.62%. With the increase of reactor speed, the molar fraction of NH_3 generated by the reaction gradually increases. In the reactor, as the reactor speed becomes lower and the temperature of the reaction process becomes lower, the N_2 oxidation time becomes shorter, and the less the production of NH_3. When the rotation speed is 89.5 r/min, the highest temperature of the reaction is too low, so NH_3 is not generated.

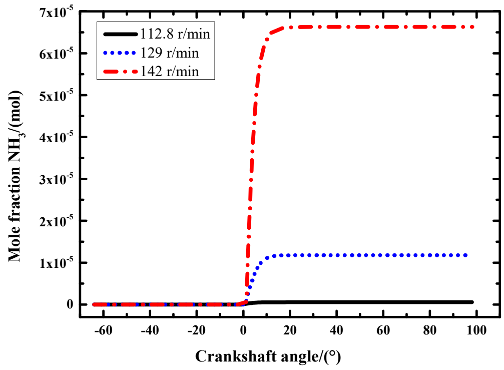

Fig 5. Mole fraction of NH_3 produced by the combustion of mixed fuel at different speeds

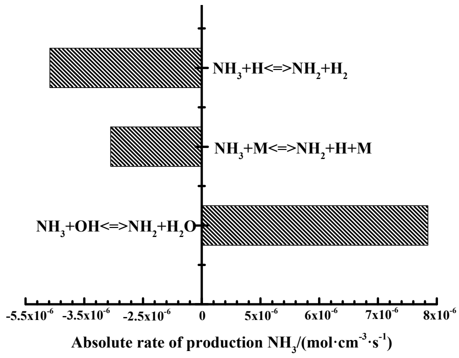

Fig 6. Main reaction equations involving NH_3 and the yield of the corresponding reaction equations

5.Conclusion

The maximum temperature in the reactor and the temperature at the opening of the exhaust port decrease with the decrease of the speed, when the ratio of CH_4 to $C_4H_{10}O$ is 6:4 and the excess air coefficient is 1.5. Compared with 142 r/min, the maximum temperature at 89.5 r/min is reduced by 28.49%, and the exhaust temperature is reduced by 58.67%. With the decrease of rotational speed, the molar fraction of NO and NH_3 at exhaust port opening decreases. By analysing the reaction mechanism at a rotation speed of 129 r/min, it can be seen that the decrease in the molar fraction of NO at a crank angle of 5°~98° is mainly consist of the partial conversion of NO to N, N_2O, NNH, and HNO, respectively. Compared with 142 r/min, the molar fraction of NO at 129 r/min decreased by 28.49%. The increase of NH_3 mole fraction at crank angle of 0°~98° is mainly due to the conversion of NH_2. Compared with 142 r/min, the NH_3 mole fraction at 129 r/min decreases by 28.49%. Therefore, reducing the speed of the diesel engine can effectively reduce the maximum temperature and the exhaust temperature, The proportional mixture of $C_4H_{10}O$ and CH_4 does not change the nature of combustion. and then decreases with the decrease of rotational speed, the production of nitrides also decreases, which further reduces pollution. Renewable energy like n-butanol is expected to be more widely used in the shipping industry in the future, to reduce nitrogen oxide emissions.

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