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Simulation of Inner-Engine NOx Emission Control on Pure Hydrogen Engines

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Abstract

Hydrogen is an ideal engine fuel. Pure hydrogen engines do not produce CO and HC emissions but face the high NOx emission problem. Inner-engine control and outer-engine control are two ways to decrease the NOx emission. Outer-engine control mainly reduce NOx emission through selective catalytic reduction (SCR), which has been well studied. However, there are few studies on NOx emission control of pure hydrogen engines through inner-engine control. In this paper, the closed homogeneous reactor (CHR) in Chemkin Pro was used to simulate the main inner-engine NOx emission control in pure hydrogen engines. The results show that single exhaust gas recirculation (EGR） decreases NOx emission by 45.3% at an EGR ratio of 20%，indicating that the NOx emission is not significantly reduced. However, EGR plus lean-burn decreases NOx emission by 96.31% at a λ of 1.4 and an EGR ratio of 20%， achieving ultra-low NOx emission of pure hydrogen engines. Compared with single EGR and EGR plus lean-burn, SNCR are better for NOx emission control. A NH3 ratio of only 10% can decrease NOx emission by 96.32% on pure hydrogen engines, while a NH3 ratio of 15% can achieve zero NOx emission on pure hydrogen engines without a large λ value and EGR ratio. However, it is necessary to accurately control the NH3 ratio in the cylinder, otherwise it is easy to produce residual NH3 which can pollute the environment.

Keywords: pure hydrogen engine； NOx emissions； lean-burn； selective non-catalytic reduction (SNCR)； exhaust gas recirculation (EGR)

1. Introduction

The massive consumption of fossil energy has brought severe pollution problem [1-2]. Seeking clean and efficient renewable energy could solve the pollution problem and alleviate energy crisis ［3-4］. Hydrogen is a kind of renewable fuel whose only combustion product is water, which will not cause any damage to the environment ［5-6］. Pure hydrogen on engines can almost completely remove CO, CO_2, unburned HC emissions, and output higher power than pure gasoline. But NOx emission is the main disadvantage of pure hydrogen engine ［7］. In order to solve the problem of NOx emission, the exhaust gas recirculation (EGR) technology, the EGR plus lean burn technology, the selective non-catalytic reduction （SNCR） technology, and the selective catalytic reduction (SCR) technology, are currently the main technical means to reduce NOx emission ［8-10］. Outer engine control mainly reduces NOx emission through SCR, which has been well studied. The EGR technology, the EGR plus lean-burn technology, and the SNCR technology are the main means of inner engine NOx emission control at present. However, there are few studies on NOx emission control of pure hydrogen engines through inner-engine control.

Therefore, this paper simulated and compared three main inner-engine NOx emission control means of pure hydrogen engines, providing theoretical basis for the choice of technical means on inner-engine to reduce NOx emission of pure hydrogen engines.

2. Simulation setup and procedure

The simulation software used in this simulation was Chemkin Pro, and the model was closed homogeneous reactor （CHR）. The H2 combustion mechanism used in this simulation was the detailed mechanism of hydrogen combustion， the NOx generation mechanism used the improved version of Zeldovitch-mechanism, and the NOx desorption mechanism is provided by Golovitchev [11-15]. All the chemical reaction mechanisms in the simulation were verified by extensive experiments， and the experimental results could match the simulation accurately. This simulation simulated three inner engine NOx emission control technical means EGR, lean-burn plus EGR and SNCR. In this experiment， five λ values(1, 1. 1, 1. 2, 1. 3, 1. 4）, five EGR ratios （0, 5%, 10%, 15%, 20%） and five NH3 ratios（0, 5%, 10%, 15%, 20%）were set. The EGR ratio is defined in Equation（1）， and the NH3 ratio is defined in Equation（2）. Tab. 1 shows the initial conditions for the closed homogeneous reactor. Vx represented the volume of x in the following equations.

Tab.1 Initial conditions for closed homogeneous reactor

Parameters	Values
Simulation time/s	0. 04
Initial temperature/K	1000
Initial pressure/MPa	0.1
mixture（. vol）	$\varphi(H_2)$ =100%
Oxidizer mixture（. vol）	$\varphi(O_2)$ =21%, $\varphi(N_2)$ =79%
Added species	H_2O；N_2；NH_3
Excess air ratio	1, 1. 1, 1. 2, 1. 3, 1. 4

3. Results and discussion

3. 1 Effect of EGR on NOx emission

Fig. 1 shows the effect of EGR on total NOx production rate and NOx emission. As can be seen from Fig. 1, with the increase of the EGR ratio, the peak value of the total NOx production rate and the total NOx emission decrease. When the EGR ratio increases from 0% to 20%， the peak value of the total NOx production rate decreases by 38. 52%, 63. 93%, 80. 33%, and 89. 34%, respectively. The total NOx emissions decrease by 11. 42%, 22. 82%, 34. 18%, and 45. 30%. The NOx formation conditions are high temperature, oxygen enrichment, and high temperature duration. On the one hand, the increase of the EGR ratio reduces the temperature in the cylinder, and at the same time, the increase of the EGR rate also dilutes the concentration of N_2 and O_2, and reduces the NOx generation rate. Therefore, the use of the EGR technology can effectively reduce NOx emission generated during hydrogen combustion.

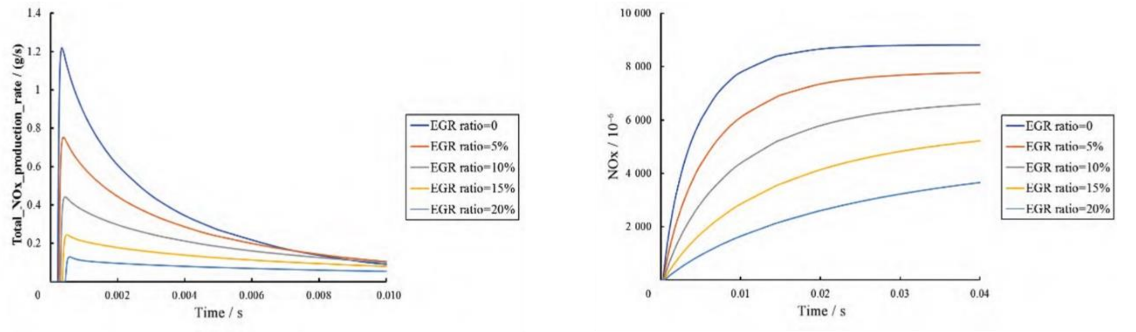

Fig.1 Effect of EGR on total NO_x production rate and NO_x emission

3. 2 Effect of EGR plus lean-burn on NOx emission

The EGR ratio was kept at 20% and the excess air ratio was increased from 1 to 1. 4 to observe the effect of EGR plus lean-burn on NOx emission. Fig. 2 shows the effect of EGR plus lean-burn on total NOx production rate and NOx emission. It can be observed that the peak value of the total NOx production rate decreased continuously with the increase of λ, but the NOx emission increases first and then decreases when λ increases. At a λ of 1. 1, the NOx emission is the highest. Although lean-burn could lower the combustion temperature, a larger λ leads to an increase of O_2 and creates favorable conditions for the oxygen enrichment, which is conducive to the generation of NOx. The increase in oxygen results in the fact that the combination of an EGR ratio of 20% with a λ of less than 1. 3 cannot effectively reduce the NOx emission. The NOx emission can be reduced by 96. 31% when λ is 1. 4 and the EGR ratio is 20%.

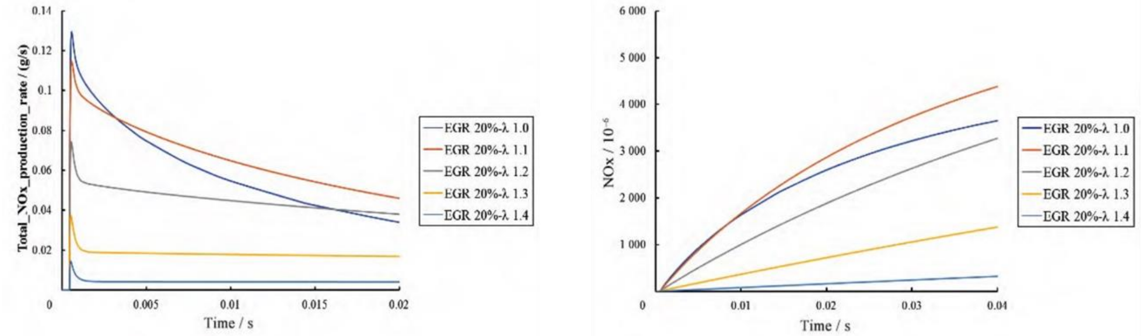

Fig.2 Effect of EGR plus lean-burn on total NO_x production rate and NO_x emission

3. 3 Effect of NH_3 on NOx emission

Fig. 3 shows the effect of NH_3 on total NOx production rate and NOx emission. It can be observed that both the positive or negative peak value of the total NOx production rate decrease continuously with the NH_3 ratio increasing, but the NOx emission decreases with the NH_3 ratio increasing.

In addition, a larger NH_3 ratio would lead to a later peak value of the total NOx production rate. When the NH_3 ratio is 10%, the NOx emission decreases by 96. 32% than without NH_3 addition while when the NH_3 ratio is large than 15%, pure hydrogen engines could achieve no NOx emission. However, a large NH3 ratio is not recommended, because a large amount of residual NH_3 will overflow, causing serious pollution to the environment.

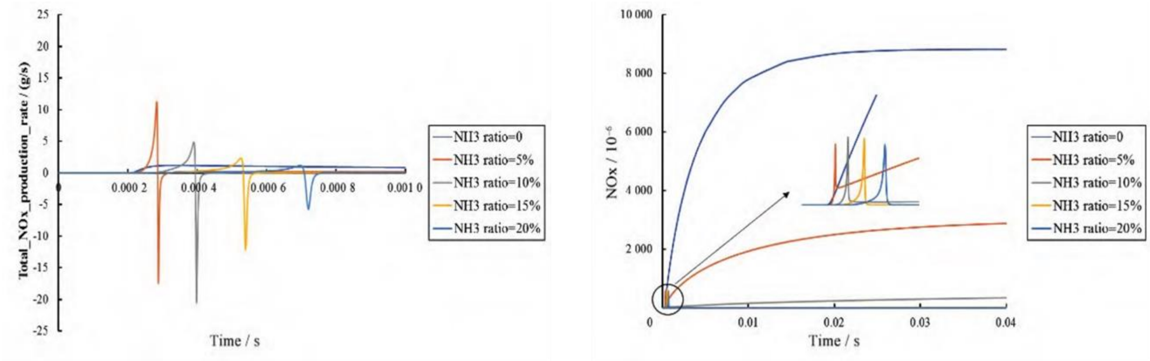

Fig.3: Effect of NH3 on total NOx production rate and NOx emission

4. Conclusions

This paper used the CHR module in CHEMKIN Pro to simulate the three main means of inner-engine NOx emission control on pure hydrogen engines, providing theoretical guidance for pure hydrogen engines to choose NOx purification means. The main results are as follows :

- EGR reduces the NOx emission generated during hydrogen combustion. The NOx emission is reduced only by 45. 3% when the EGR ratio is 20%. Therefore, to achieve ultra-low NOx emission using pure hydrogen engines by adopting the EGR technology, a larger EGR ratio or EGR in combination with external purification should be used.
- Compared with single EGR, EGR plus lean-burn is more efficient in reducing the NOx emission by using pure hydrogen engines. Pure hydrogen engines need a large EGR ratio and λ value. The NOx emission can be reduced by 96. 31% when λ is 1. 4 and the EGR ratio is 20%, achieving ultra-low NOx emission of pure hydrogen engines. To control NOx emissions by using pure hydrogen engine and EGR plus lean-burn, the engine condition monitoring should be strengthened to avoid misfire because of the large EGR ratio and λ value.
- Compared with EGR, and EGR plus lean burn, SNCR is better in inner-engine NOx emission control, because it requires only a NH3 ratio of 10% to achieve ultra-low NOx emissions on pure hydrogen engines. A NH3 ratio a 15% can make pure hydrogen engines achieve zero NOx emission.

SNCR avoids pure hydrogen engines having to operate under a large λ and EGR ratio to decrease NOx emission, avoiding the power loss of pure hydrogen engines, making combustion more stable. In the control of NOx emission of pure hydrogen engines, SNCR should be the main technical means to be adopted, and zero emission can be achieved when the proportion of NH3 is controlled reasonably.

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