第 49 卷第 S1 期
2021 年 12 月

同济大学学报(自然科学版)
JOURNAL OF TONGJI UNIVERSITY(NATURAL SCIENCE)

Vol. 49 No. S1
Dec. 2021

文章编号：0253-374X(2021)S1-0079-04

DOI：10. 11908/j. issn. 0253-374x. 22785

纯氢内燃机氮氧化物排放机内净化的仿真研究

李德成，杜耀东，于秀敏
（吉林大学 汽车工程学院，长春 130022）

摘要：纯氢内燃机工作时不会产生一氧化碳、碳氢化合物等有害排放物，但会面临高氮氧化物排放的问题，而机内净化和机外净化是控制氮氧化物排放的两种常用手段。机外净化主要通过成熟的选择性催化还原(SCR)技术降低氮氧化物排放，但机内净化技术目前还很少被关注。为此，采用Chemkin Pro软件中的闭口均质反应器模型来模拟纯氢内燃机氮氧化物排放的机内净化。结果显示，废气再循环(EGR)技术可以降低氮氧化物排放，当EGR率为20%时，氮氧化物排放降低了45.3%，但仅使用EGR来降低氮氧化物排放的效果还不够明显，氮氧化物排放依然很高。与单独应用EGR技术相比，EGR技术与稀薄燃烧技术相结合能够更好地实现氮氧化物排放控制，如过量空气系数为1.4、EGR率为20%时，氮氧化物排放量降低了96.31%，实现了纯氢发动机的超低排放。与EGR技术以及EGR-稀薄燃烧技术相比，内部选择性非催化还原技术的氮氧化物排放控制效果更佳，仅10%的氨气比例就能使纯氢发动机氮氧化物排放降低96.32%，15%的氨气比例可以实现纯氢发动机氮氧化物零排放，且并不需要EGR或稀薄燃烧技术的参与；然而，精确控制发动机缸内氨气比例是十分必要的，否则会产生残氨排放污染环境。

关键词：纯氢内燃机；氮氧化物排放；稀薄燃烧；选择性非催化还原；废气再循环

中图分类号：TK46+3　　　　**文献标志码**：A

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

LI Decheng, DU Yaodong, YU Xiumin
(College of Automotive Engineering, Jilin University, Changchun 130022, China)

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 NO_x emission. Outer-engine control mainly reduce NO_x emission through selective catalytic reduction (SCR), which has been well studied. However, there are few studies on NO_x 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 NO_x emission control in pure hydrogen engines. The results show that single exhaust gas recirculation (EGR) decreases NO_x emission by 45.3% at an EGR ratio of 20%, indicating that the NO_x emission is not significantly reduced. However, EGR plus lean-burn decreases NO_x emission by 96.31% at a λ of 1.4 and an EGR ratio of 20%, achieving ultra-low NO_x emission of pure hydrogen engines. Compared with single EGR and EGR plus lean-burn, SNCR are better for NO_x emission control. A NH_3 ratio of only 10% can decrease NO_x emission by 96.32% on pure hydrogen engines, while a NH_3 ratio of 15% can achieve zero NO_x emission on pure hydrogen engines without a large λ value and EGR ratio. However, it is necessary to accurately control the NH_3 ratio in the cylinder, otherwise it is easy to produce residual NH_3 which can pollute the environment.

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

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 NO_x emission is the main disadvantage of pure hydrogen engine[7]. In order to

收稿日期：2021-09-25
第一作者：李德成(1995—)，男，博士生，主要研究方向为内燃机燃烧与排放控制技术。E-mail：342810078@qq. com
通信作者：杜耀东(1989—)，男，讲师，工学博士，主要研究方向为纯氢内燃机燃烧与控制技术。E-mail：duyd2021@jlu. edu. cn

solve the problem of NO_x 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 NO_x emission[8-10]. Outer-engine control mainly reduces NO_x 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 NO_x emission control at present. However, there are few studies on NO_x emission control of pure hydrogen engines through inner-engine control. Therefore, this paper simulated and compared three main inner-engine NO_x emission control means of pure hydrogen engines, providing theoretical basis for the choice of technical means on inner-engine to reduce NO_x emission of pure hydrogen engines.

1 Simulation setup and procedure

The simulation software used in this simulation was Chemkin Pro, and the model was closed homogeneous reactor (CHR). The H_2 combustion mechanism used in this simulation was the detailed mechanism of hydrogen combustion, the NO_x generation mechanism used the improved version of Zeldovitch-mechanism, and the NO_x desorption mechanism is provided by Golovitchev[11-13]. 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 NO_x 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 NH_3 ratios (0, 5%, 10%, 15%, 20%) were set. The EGR ratio is defined in Equation (1), and the NH_3 ratio is defined in Equation (2). Tab. 1 shows the initial conditions for the closed homogeneous reactor. V_x 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
Fuel 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

$$\text{EGR}\ ratio=\frac{V_{\text{EGR}}}{V_{\text{EGR}}+V_{\text{AIR}}+V_{\text{H}_2}} \tag{1}$$

$$\text{NH}_3\ ratio=\frac{V_{\text{NH}_3}}{V_{\text{NH}_3}+V_{\text{AIR}}+V_{\text{H}_2}} \tag{2}$$

2 Results and discussion

2.1 Effect of EGR on NO_x emission

Fig. 1 shows the effect of EGR on total NO_x production rate and NO_x emission. As can be seen from Fig. 1, with the increase of the EGR ratio, the peak value of the total NO_x production rate and the total NO_x emission decrease. When the EGR ratio increases from 0% to 20%, the peak value of the total NO_x production rate decreases by 38.52%, 63.93%, 80.33%, and 89.34%, respectively. The total NO_x emissions decrease by 11.42%, 22.82%, 34.18%, and 45.30%. The NO_x 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 NO_x generation rate. Therefore, the use of the EGR technology can effectively reduce NO_x emission generated during hydrogen combustion.

2.2 Effect of EGR plus lean-burn on NO_x 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 NO_x emission. Fig. 2 shows the effect of EGR plus lean-burn on total NO_x production rate and NO_x emission. It can be observed that the peak value of the total NO_x production rate decreased continuously with the increase of λ, but the NO_x emission increases first and then decreases when

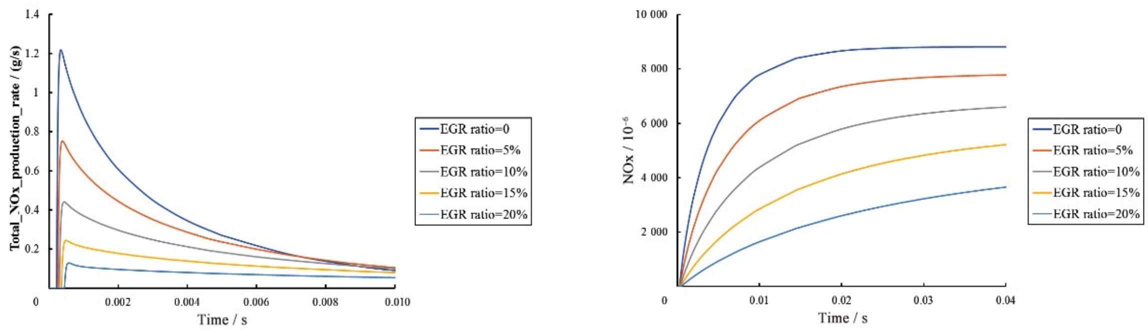

Fig.1　Effect of EGR on total NO_x production rate and NO_x emission

λ increases. At a λ of 1.1, the NO_x 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 NO_x. 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 NO_x emission. The NO_x emission can be reduced by 96.31% when λ is 1.4 and the EGR ratio is 20%.

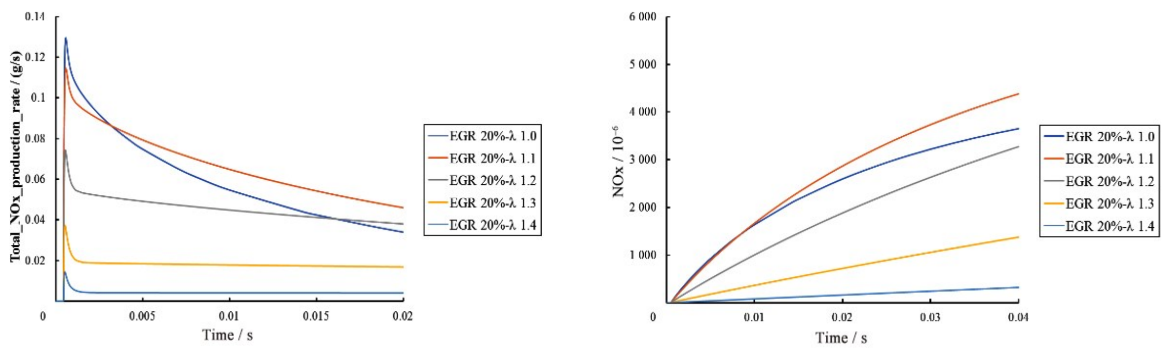

Fig.2　Effect of EGR plus lean-burn on total NO_x production rate and NO_x emission

2.3　Effect of NH_3 on NO_x emission

Fig. 3 shows the effect of NH_3 on total NO_x production rate and NO_x emission. It can be observed that both the positive or negative peak value of the total NO_x production rate decrease continuously with the NH_3 ratio increasing, but the NO_x 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 NO_x production rate. When the NH_3 ratio is 10%, the NO_x 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 NO_x emission. However, a large NH_3 ratio is not recommended, because a large amount of residual NH_3 will overflow, causing serious pollution to the environment.

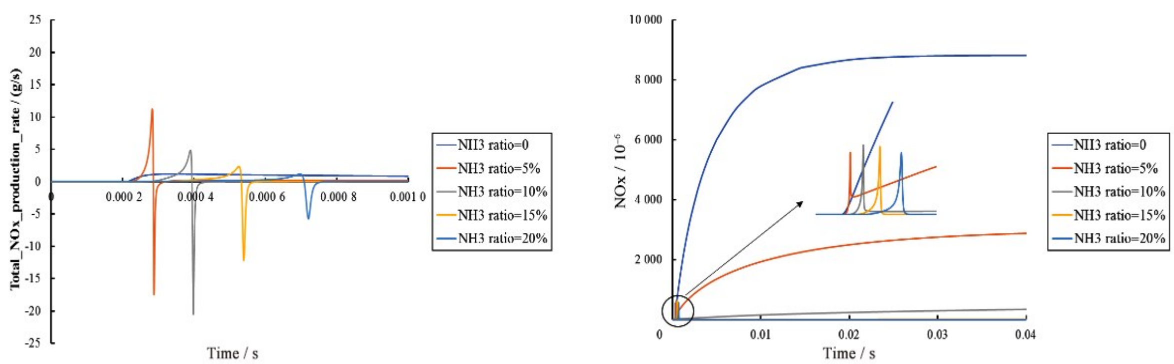

Fig.3　Effect of NH_3 on total NO_x production rate and NO_x emission

3 Conclusions

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

(1) EGR reduces the NO_x emission generated during hydrogen combustion. The NO_x emission is reduced only by 45.3% when the EGR ratio is 20%. Therefore, to achieve ultra-low NO_x emission using pure hydrogen engines by adopting the EGR technology, a larger EGR ratio or EGR in combination with external purification should be used.

(2) Compared with single EGR, EGR plus lean-burn is more efficient in reducing the NO_x emission by using pure hydrogen engines. Pure hydrogen engines need a large EGR ratio and λ value. The NO_x emission can be reduced by 96.31% when λ is 1.4 and the EGR ratio is 20%, achieving ultra-low NO_x emission of pure hydrogen engines. To control NO_x 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.

(3) Compared with EGR, and EGR plus lean-burn, SNCR is better in inner-engine NO_x emission control, because it requires only a NH_3 ratio of 10% to achieve ultra-low NO_x emissions on pure hydrogen engines. A NH_3 ratio a 15% can make pure hydrogen engines achieve zero NO_x emission. SNCR avoids pure hydrogen engines having to operate under a large λ and EGR ratio to decrease NO_x emission, avoiding the power loss of pure hydrogen engines, making combustion more stable. In the control of NO_x 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 NH_3 is controlled reasonably.

References:

[1] LI D, WANG H, YU X, *et al*. Combustion and emission characteristics of an Acetone-Butanol-Ethanol (ABE) spark ignition engine with hydrogen direct injection[J]. International Journal of Hydrogen Energy, 2021, 46(58): 30145.

[2] GONG C, YI L, ZHANG Z, *et al*. Assessment of ultra-lean burn characteristics for a stratified-charge direct-injection spark-ignition methanol engine under different high compression ratios [J]. Applied Energy, 2020, 261: 114478.

[3] ZHEN X, WANG Y. An overview of methanol as an internal combustion engine fuel[J]. Renewable and Sustainable Energy Reviews, 2015, 52: 477.

[4] THANGAVELU S K, AHMED A S, ANI F N. Review on bioethanol as alternative fuel for spark ignition engines [J]. Renewable and Sustainable Energy Reviews, 2016, 56: 820.

[5] AYAD S M M E, BELCHIOR C R P, DA SILVA G L R , *et al*. Analysis of performance parameters of an ethanol fueled spark ignition engine operating with hydrogen enrichment [J]. International Journal of Hydrogen Energy, 2020, 45(8): 5588.

[6] YU X, LI G, DONG W, *et al*. Numerical study on effects of hydrogen direct injection on hydrogen mixture distribution, combustion and emissions of a gasoline/hydrogen SI engine under lean burn condition[J]. International Journal of Hydrogen Energy, 2020, 45(3): 2341.

[7] KARTHIKEYAN S, PERIYASAMY M. Impact on the power and performance of an internal combustion engine using hydrogen[J]. Materials Today: Proceedings, 2021. https://doi.org/10.1016/j.matpr.2021.02.356.

[8] YU X, ZHAO Z, HUANG Y, *et al*. Experimental study on the effects of EGR on combustion and emission of an SI engine with gasoline port injection plus ethanol direct injection [J]. Fuel, 2021, 305: 121421.

[9] YU X, GUO Z, HE L, *et al*. Experimental study on lean-burn characteristics of an SI engine with hydrogen/gasoline combined injection and EGR [J]. International Journal of Hydrogen Energy, 2019, 44(26): 13988.

[10] HE F, YU X, DU Y, *et al*. Inner selective non-catalytic reduction strategy for nitrogen oxides abatement: investigation of ammonia aqueous solution direct injection with an SI engine model[J]. Energies, 2019, 12(14): 2742.

[11] Ó CONAIRE M , CURRAN H J, SIMMIE J M, *et al*. A comprehensive modeling study of hydrogen oxidation [J]. International Journal of Chemical Kinetics, 2004, 36(11): 603.

[12] AN H, YANG W M, LI J, *Et al*. Modeling analysis of urea direct injection on the NO_x emission reduction of biodiesel fueled diesel engines[J]. Energy Conversion and Management, 2015, 101: 442.

[13] GOLOVITCHEV V I, MONTORSI L, DENBRATT I. Numerical evaluation of a new strategy of emissions reduction by urea direct injection for heavy duty diesel engines [J]. Engineering Applications of Computational Fluid Mechanics, 2007, 1(3): 189.