

Study of Hydrogen Internal Combustion Engine Vehicles Based on the Whole Life Cycle Evaluation Method

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In order to better achieve the goal of low carbon emissions from vehicles, a whole life cycle assessment of hydrogen-fueled internal combustion engine vehicles has been conducted in recent years. Based on the study of hydrogen use around the world, we studied the emission and economic performance of hydrogen-fueled internal combustion engine vehicles from the beginning of hydrogen production to the end of use (Well-to-Wheel, WTW) based on the whole life cycle evaluation method. The results show that the overall environmental impact of hydrogen production by steam reforming of natural gas is the smallest, and that the rational use of "abandoned electricity" for hydrogen production from electrolytic water in the western part of China significantly reduces the overall environmental impact and the cost of hydrogen production. In the use phase, the emissions are less, which not only can meet the National 6 emission standard, but also can reach higher emission standard after adding exhaust gas recirculation (EGR). From the whole life cycle point of view, hydrogen-fueled internal combustion engine has a very good development prospect.

Keywords: Whole Life Cycle; Hydrogen Fuel Internal Combustion Engine; Emission; Economy

Introduction

By 2020, the number of cars in China has reached 281 million [1], which results in the problem of pollutant emissions and energy consumption. According to 2020 data, China's dependence on imported oil has reached 69.84% in 2020 [2]. Hydrogen, as a clean and renewable new energy source, can not only reduce the emission of pollutants from vehicles, but also alleviate the problem of transitional dependence on traditional energy sources.

In this study, a comprehensive evaluation of new energy vehicles fueled by hydrogen is conducted from the whole life cycle of the energy source. Most studies on the whole life cycle evaluation of hydrogen have focused on hydrogen fuel cell vehicles. Lin *et al.* [3] used the GREET model to comprehensively evaluate the CO₂ emissions of hydrogen fuel cell vehicles under various routes of hydrogen fuel production and concluded that the energy consumption and CO₂ emissions could be reduced by 90% under the clean way of hydrogen production. Chen [4], Andrew [5], and Kong *et al.* [6] studied the emissions during the production of different hydrogen production methods, and obtained the most economical and least emitting method through comparative analysis. Changing the power generation structure not only reduces the overall

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environmental impact value of electrolytic water hydrogen production, but also reduces the cost of hydrogen production. Daniele *et al.* [7] evaluated the life-cycle performance of three different types of vehicles based on wind power electrolysis of water for hydrogen production and the results showed that hydrogen fuel is an excellent decarbonization solution. Both Dong *et al.* [8] and Huang *et al.* [9] performed life cycle analysis of the environmental impact of fuel cell vehicle energy under different fossil fuel-based hydrogen fuel paths. The results showed that supplying fuel cell vehicles with hydrogen from natural gas reforming is the most advantageous in terms of energy saving and emission reduction.

Hydrogen-fueled internal combustion engines are another way to use hydrogen as an alternative energy source. Hydrogen fuel cells are hampered by materials and technology, which provides an opportunity for the development of hydrogen-fueled internal combustion engines. The use of hydrogen fuel cells involves electrochemical reactions which require the purity of the hydrogen used (usually greater than 99.99%) to minimize the impact of impurities in the hydrogen on the catalyst and electrolyte, while hydrogen-fueled internal combustion engines require low purity of hydrogen. In contrast, hydrogen internal combustion engines have a definite advantage in terms of manufacturing and fuel purification costs. There are no reports on the life cycle of hydrogen-fueled internal combustion engine vehicles in China, and few studies have been done by other countries. Halim *et al.* [10] compared gasoline doped hydrogen with pure gasoline engine and analyzed the investment cost planning of two different combustion modes in five and ten years, and the results showed that after the fourth year, the investment cost of gasoline doped hydrogen car is lower than that of pure gasoline car, and the gap increases gradually with the increase of service life. However, the main study focuses on the consumption in the hydrogen production phase, and does not analyze the emissions and energy consumption in the combustion phase, which is not a comprehensive evaluation. In summary, the study of the whole life cycle of hydrogen fueled internal combustion engines not only reveals the application prospects of hydrogen fueled internal combustion engines, but also makes the evaluation of hydrogen fuel in vehicles more comprehensive.

Research Methods and Contents

Whole Life Cycle Evaluation Method

Life cycle evaluation method is a method of aggregating and evaluating one or more specific indicators of a product (service) system throughout its life cycle in terms of all inputs, outputs, and their direct or indirect impacts on the external environment [11]. The life cycle assessment of vehicles can be described as a well-to-wheel (WTW) process, which can be divided into two stages: well-to-tank (WTT) and tank-to-wheel (TTW). The hydrogen-fueled internal combustion engine can be described as the stages of hydrogen production, transportation, and use of hydrogen fuel in the internal combustion engine. The system boundary is shown in Figure 1.

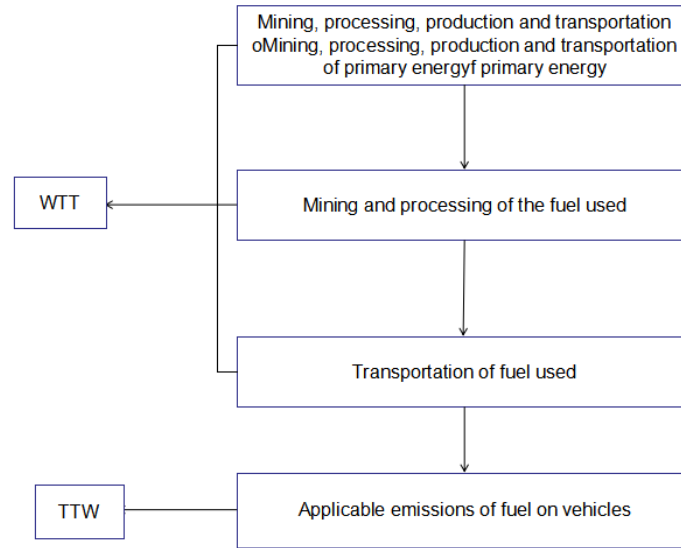


Figure 1. Hydrogen fuel system boundary

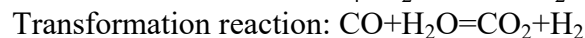
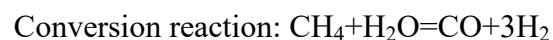
Research Content

This study focuses on the whole life cycle analysis of a hydrogen-fueled internal combustion engine by selecting the two most and least energy-consuming and emission-consuming ways to produce hydrogen from a variety of hydrogen production methods, and considering the whole life cycle of hydrogen from the generation of hydrogen to the end of its emission after use in a hydrogen-fueled internal combustion engine, focusing on the production, manufacturing, and use costs (*i.e.*, understood the economics) and the emission of pollutants (mainly NO_x and CO_2 -based emissions). Because only a simple modification of a conventional gasoline engine is needed to burn hydrogen and the weight of the vehicle manufacturing process itself is less than 1% [12], in order to study the main content, the vehicle manufacturing process is ignored and only the energy consumption and pollutant emissions during the production and manufacturing costs of hydrogen fuel and its use in the vehicle are focused.

Two-stage Energy Consumption and Emissions

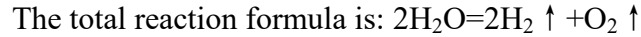
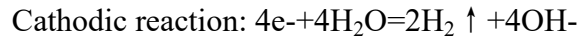
Hydrogen Production Method

1. Hydrogen production by steam reforming of natural gas: The basic principle of producing hydrogen from natural gas is to use natural gas, high-temperature steam and synthetic reaction to form a mixture of hydrogen (H_2), carbon monoxide (CO) and a small amount of carbon dioxide (CO_2). CO reacts with water again to produce additional hydrogen. Hydrogen production by steam reforming of natural gas is the most effective and common hydrogen production technology. The chemical reaction formula are as follows:



2. Hydrogen production by water electrolysis: The principle of hydrogen production by water electrolysis is electrochemical reaction which uses direct current to

electrolyze the electrolyte, and chemical reactions that occur at the two ends of different electrodes, thereby producing hydrogen and oxygen at the cathode and anode, respectively. The chemical reaction formula is as follows:



3. Coke oven gas hydrogen production method: Coke oven gas is a hydrogen-rich combustible gas. Using coke oven gas after removing impurities, the pressure swing adsorption separation method can be used to produce hydrogen.

In order to study the value of the entire hydrogen energy production range, this research selects hydrogen production by steam reforming of natural gas and electrolysis water hydrogen production methods for research.

Energy Consumption and Emissions in WTT Phase

Energy Consumption for Hydrogen Production

The consumption of one cubic meter of hydrogen produced under standard conditions (the quantities of reactants and products involved in the following are standard conditions) is analyzed. The cost of hydrogen production mainly includes natural gas costs, deionized water costs, cooling water costs, and electricity costs. For the four parts, the prices of raw materials are based on the relevant standards and related documents [13-14] announced by Beijing in 2021:

Table 1. Consumption and unit price of raw materials for producing 1 cubic meter of hydrogen (Unit : Yuan ¥)

	Natural gas steam Reforming hydrogen production	Electrolyte Hydrogen production	Unit price
Natural gas/m ³	0.48	0.00	4.25
Deionized water/kg	1.30	0.88	0.069
Cooling water/kg	6.00	3.00	0.003
Electricity/degree	0.40	5.50	0.25
Equipment depreciation	0.1583	0.1286	-

Based on the data in Table 1, the costs for producing 1 cubic meter of hydrogen via steam reforming of natural gas and electrolysis of water are 2.37604 and 2.14474 yuan, respectively. From the perspective of production costs, the cost of hydrogen production from electrolysis of water is lower, which is 9.61% lower than that of natural gas reforming.

Hydrogen Production Emissions

(1) Emissions from hydrogen production by steam reforming of natural gas

Natural gas is a primary energy source. The main components are methane and a small amount of olefins. There is no harmful gas emission during the acquisition process, but CO₂ is emitted during the hydrogen production process.

(2) Discharge of hydrogen production by electrolysis of water

There will be no emissions of pollutants in the process of electrolysis of water to produce hydrogen. But if considering that thermal power generation accounts for 73.32%

of the total power generation of china, pollutants are emitted during the power generation process.

Comparison of Two Hydrogen Production Schemes

Table 2. Energy consumption and emissions of the two hydrogen production schemes

	Natural gas reforming to produce hydrogen	Hydrogen production by electrolysis of water
Coal/kg	0.000	0.320
CH ₄ /m ³	0.480	0.000
CO/kg	0.005	0.136
CO ₂ /kg	0.491	1.030
NO _x /kg	0.007	0.015
SO ₂ /kg	0.007	0.030
PM2.5/kg	0.001	0.081

Table 2 shows the energy consumption and emissions of two different hydrogen production schemes to produce 1 cubic meter of hydrogen. Using CML2001 [15] to normalize and quantify the above data, the comprehensive environmental impact value is shown in Table 3:

Table 3. Comprehensive environmental impact values of the two hydrogen production schemes

Plan	Natural gas reforming to produce hydrogen	Hydrogen production by electrolysis of water
Comprehensive environmental impact value	4.8×10^{-11}	2.99×10^{-9}

The comprehensive environmental impact value of hydrogen production by steam reforming of natural gas is only 1.6% of that of hydrogen production by electrolysis of water, and its impact on the environment is much smaller than that of hydrogen production by electrolysis of water, mainly because the electricity consumed comes from thermal power generation.

Scenario Simulation

The proportion of thermal power generation in western china is less than 15%. Table 4 shows the power generation structure of the four western regions in China in 2020.

Table 4. Power generation structure of Sichuan, Yunnan, Tibet and Qinghai in China in 2020

Source Province	Sichuan	Yunnan	Tibet	Qinghai
Thermal power	13.69%	9.51%	3.62%	13.5%
Hydropower	83.78%	81.97%	89.31%	65.78%
wind power	1.99%	7.54%	0.88%	6.53%
Solar energy	0.54%	0.98%	6.09%	14.19%
total	100%	100%	100%	100%

For different power generation structures, the comprehensive environmental impact values of the above four places can be calculated through the GaBi model. The comprehensive environmental impact results of the electrolytic water method in different power generation structures are shown in Table 5.

Table 5. Comprehensive environmental impact value of electrolyzed water in four provinces

Province	Sichuan	Yunnan	Tibet	Qinghai
Comprehensive environmental impact value	3.2×10^{-10}	2.9×10^{-10}	1.6×10^{-10}	3.1×10^{-10}

The use of electrolyzed water to produce hydrogen in western china has less impact on the environment than the use of electrolyzed water to produce hydrogen in other cities in China. As can be seen from Tables 3 and 5, although there is still a gap compared with hydrogen production by steam reforming of natural gas, the overall environmental impact has been reduced from 62 times to 3.3 times. Since the unstable power generation of renewable energy has impacted the grid, causing grid fluctuations and insecurity, this part of the power that cannot be connected to the grid has caused a large amount of "power abandonment". Table 6 shows the statistics of china's "abandonment of electricity" in recent years.

Table 6. 2017-2020 National abandoned electricity in China

Type Years	Abandon water	Abandon light	Abandon the wind
2017	4%	6%	12%
2018	5%	3%	7.2%
2019	4%	2%	4%
2020	3.39%	2%	3%

Energy Consumption and Emissions in TTW Phase

Starting from the hydrogen fuel internal combustion engine, the energy consumption and emissions of the TTW phase are analyzed. The AVL-Fire three-dimensional simulation software is used for simulation. The model is based on a hydrogen-fueled internal combustion engine modified from the Jialing JH-600 single-cylinder engine. In order to ensure the reliability of the test simulation, the experimental data and the simulation data were compared at 3000 r/min and the equivalent ratio of 0.4. The simulated value is slightly higher than the experimental value, mainly because the simulated working conditions are relatively ideal. It is believed that the cylinder is fully enclosed, and there will be some deviations in the experiment. The maximum difference is 1.2%. It can be considered that this model can well reflect the actual working conditions of the hydrogen fuel internal combustion engine.

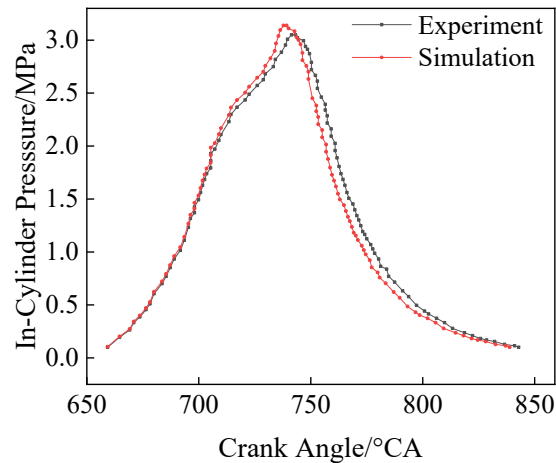


Figure 2. Model validation

Energy Consumption

Hydrogen has high thermal efficiency whether used as the power source of hydrogen fuel cell or hydrogen fuel internal combustion engine. The low calorific value of hydrogen is 119.64 MJ/kg, which is 2.72 times that of gasoline. The combustion speed of hydrogen is fast, and high thermal efficiency [16]. BMW was the first company to develop hydrogen-fueled internal combustion engine vehicles. As early as 2004, BMW Motor Company conducted tests. The test result is that the hydrogen consumption per 100 kilometers is 3.7 kg, which is equivalent to 13.8 L gasoline/100-km. The hydrogen consumption can be reduced to 2.1 kg hydrogen/100-km at high speed, which is equivalent to 7.8 L gasoline/100-km [17]. Based on a 2.0-L gasoline engine modified hydrogen fuel internal combustion engine test, Beijing Institute of Technology Sun Baigang and others found that when the vehicle speed reaches 80 km/h, the hydrogen consumption per 100 kilometers is 1.43 kg. When the vehicle speed decreases, the hydrogen consumption per 100 kilometers drops to 1.27 kg, equivalent to 4.7 L gasoline/100-km, which is 18.9% lower than the original engine fuel consumption [18].

Through simulation, the fuel consumption and indicated thermal efficiency of hydrogen-fueled internal combustion engines under different operating conditions are studied. Figure 3 shows that the maximum power speed of the modified hydrogen fuel internal combustion engine is 6000 r/min. From the simulation results, it can be seen that at a hydrogen injection pressure of 4.5 bar, the maximum power at an equivalent ratio of 1.05 can reach 25 kW, and the maximum hydrogen consumption is 2.124 kg Hydrogen/h which is equivalent to 7.86 L gasoline/h. It can be seen from Figure 3 that as the engine speed increases, the indicated thermal efficiency of the hydrogen fuel internal combustion engine first increases and then decreases. The maximum indicated thermal efficiency can reach 43.2% at 3000 r/min. Compared with the maximum output power of 30 kW of the original engine, the maximum power of the modified hydrogen fuel internal combustion engine is reduced by 16.7%, but the indicated thermal efficiency can reach up to 43.2%, which is a great improvement compared with the traditional gasoline engine.

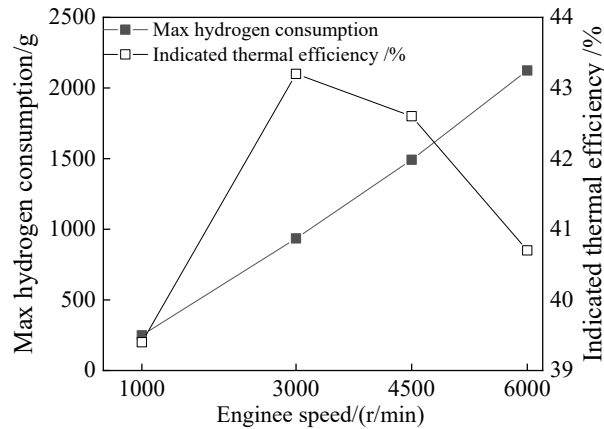


Figure 3. Maximum hydrogen consumption and indicated thermal efficiency at different speeds

Emissions

Hydrogen is a clean energy source. There are few pollutant emissions during the combustion process. Compared with traditional internal combustion engines, the emissions of unburned hydrocarbon are almost negligible. Compared with traditional internal combustion engines, the emission of greenhouse gases can be reduced by 90%. The main pollutant is nitrogen oxides. In recent years, research on technologies for reducing nitrogen oxide emissions has become more and more mature, usually using exhaust gas recirculation (EGR) technology and in-cylinder water injection.

The simulation simulates the combustion emissions of the engine at 4 speeds and 5 loads. Table 7 shows the specific parameter levels:

Table 7. Simulation scheme

parameter	level				
Rotating speed rpm	1000	3000	4500	6000	
Load	10%	30%	50%	70%	100%
Equivalent ratio	0.5	0.6	0.7	0.84	1.05

Table 8 shows the simulation results of nitrogen oxide emissions at different speeds and loads.

Table 8. The mass fraction of NO under different working conditions (unit: ppm)

Equivalent ratio \ Rotational Speed	0.5	0.6	0.7	0.84	1.05
1000r/min	6	32	956	1969	195
3000r/min	60	895	4064	4985	365
4500r/min	159	2362	6256	6958	569
6000r/min	269	3025	6589	7846	695

The data in Table 8 are NO emissions under all operating conditions. When the normal working speed is below 3000 r/min and the equivalent ratio is lower than 0.5 and higher than 1.05, the NO emission is below 500ppm. At high speed and medium and high load (0.67-0.84), NO emission increases sharply. Compared with traditional internal combustion engine exhaust gas treatment devices that need to reduce CO, unburned hydrocarbons (HC) and NO emissions, the exhaust gas treatment of hydrogen fuel internal combustion engines only needs to reduce NO emissions. The simplest technology to reduce high-load NO emissions is the EGR Technology. Table 9 shows the NO

emission after adopting the EGR technology, in which 1000 r/min adopts 5% EGR, and the remaining speed is 10% EGR.

By comparing Table 8 and Table 9, it can be found that the highest reduction in NO emissions after the use of EGR technology has reached 94.1%. At 1000 r/min and 3000 r/min speeds, it is lower than 50 ppm at full load and low load, which is close to zero emission. The main reasons for the reduction of NO emissions are: increasing EGR reduces the fresh charge in the combustible mixture, the maximum combustion temperature in the cylinder decreases, the high temperature duration decreases, and the optimal NO generation conditions are changed. 4500 r/min and 6000r/min are the highest torque speed and the highest power speed. The NO emission is higher under medium and high loads, but the frequency of use is low. If you need to work at this speed for a short time, you can appropriately sacrifice the output power and the use of 15% EGR can reduce NO emissions by 92.6%, and it is also less than 500 ppm under medium and high loads.

Table 9. NO emissions (ppm) under different working conditions after using EGR

Rotational Speed	Equivalent ratio				
	0.5	0.6	0.7	0.84	1.05
1000r/min	0.4	1.9	58.7	210.3	11.7
3000r/min	3.5	53.7	243.6	485.6	21.9
4500r/min	39.8	590.5	1564	1739.5	142.2
6000r/min	67.2	756.3	1647.3	1961.5	173.8

Table 10. Emission test of hydrogen fuel internal combustion engine

Projects	Emissions/(g/km)		
	CO	HC	NOx
CHINA 6	0.7	0.068	0.05
Simulation results	0.09	0.033	0.042

Table 10 shows the various emissions after increasing EGR. According to limits and measurement methods for emissions from light-duty vehicles (CHINA 6). Carbon monoxide emissions are only 12.8% of the regulations, HC emissions are 48.5% of the regulations, and nitrogen oxides emissions are slightly higher, at 84% of the regulations.

In addition to adding exhaust gas treatment equipment, there are many ways to reduce nitrogen oxides. (1) Hydrogen has a wide range of flammable limits, and controlling the equivalent ratio below 0.5 or above 1.05 can effectively reduce NO emissions; (2) It is possible to mix hydrogen and natural gas to reduce nitrogen oxides at the expense of low carbon emissions Emissions.

CONCLUSIONS

(1) The comprehensive environmental impact of hydrogen production by steam reforming of natural gas is only 1.6% of that of hydrogen production from electrolyzed water; in western china, "abandonment of electricity" is used to produce hydrogen from electrolyzed water, and the cost of hydrogen production from electrolyzed water is only 1/10 of that from natural gas reforming.

(2) The hydrogen consumption per hundred kilometers of the modified hydrogen internal combustion engine is 12.3% lower than the fuel consumption of the original gasoline engine without modification.

(3) The NO_x emission of hydrogen fuel internal combustion engine is greatly reduced under the working conditions of equivalent ratio less than 0.5 and higher than 1.05. Under the coordination of EGR technology under medium and high loads, it can easily reach the national VI emission standards and there is room for further improvement.

Conflict of Interest

The authors declare that there is no conflict of interests regarding the publication of this paper.

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