Computational and analytical evaluation of the efficiency of using hydrogen as a fuel in an internal combustion engine

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Abstract. There are reasons to look for alternative sources of fuel because of the automobile industry development. Firstly, oil is a mined, not a produced fuel, sooner or later it will run out. According to various statistical sources, known deposits are gradually being depleted. Another important problem is air pollution caused by road transport. Most of the existing cars run on gasoline and diesel engines that burn oil to get the car going. Combustion of hydrocarbons that make up oil releases a large amount of harmful substances, in particular, particulate matter and volatile organic compounds. Using hydrogen as an alternative fuel can solve the problem of finding new oil fields, and also, due to the absence of emissions into the atmosphere, it can solve the problem of air pollution. The article presents a brief history of the development of engine building and a description of hydrogen technologies in engines. The article presents a computational and analytical assessment of the efficiency of using hydrogen fuel in an internal combustion engine in relation to the bus fleet of the Yekaterinburg city. It was found that the conversion of a gasoline engine to hydrogen fuel leads to a decrease in specific fuel consumption by 20% (at the nominal mode). It is shown that the payback period for the transfer of 20 buses to hydrogen is about 8 years.

1. Introduction
The first hydrogen-fueled internal combustion engine (ICE) was invented by François Isaac de Rivaz in 1806. In Russia, such installations were first used in 1941 during the siege of Leningrad, and already in the 80s, in addition to the USSR, such engines have been developed in some European countries, the USA and Japan. Initially, the hydrogen engine had a very complex design. The connecting rod-piston system was spark-ignited. The ignition of a mixture of hydrogen and oxygen with an electric spark set the cylinder in motion. The ignition had to be generated manually when the piston was lowered. Two years later, de Rivaz developed a hydrogen-powered plant. The installation moved independently. As a prototype, Russian inventors used an engine from a GAZ-AA car. The principle of operation differed from the French analogue: From a hydrogen balloon lowered to the ground, hydrogen is pumped into a gas tank located in the foreground. Gaseous fuel from the gasholder with spent hydrogen is supplied through a flexible hose to the internal combustion engine of the GAZ-AA car [1-2].

Oil is mined, not produced fuel, sooner or later it will run out. This is a reason to find an alternative source of fuel. It is obvious that the known deposits are gradually being depleted. The existing methods for estimating reserves are not entirely correct and depend on several factors:

- The quality of the oil has not yet been discovered. Such oil may not be usable.
If the quality of the oil is suitable for use, the depth of the location of this oil is large enough. Extraction in this case will be costly and this will lead to an even greater increase in oil prices [3].

Also, an important problem is that cars run on fuel that contains a large amount of petroleum products. Combustion of these petroleum products produces exhaust gases. Most cars run on gasoline and diesel engines that burn oil to get the car going. As you know, during the combustion of hydrocarbons that make up oil, a large amount of harmful substances is released, in particular, solid particles and volatile organic compounds, which accumulate in the atmospheric air in large quantities. 40-75% of air pollution is accounted for by gasoline engines [4-5].

The use of hydrogen as an alternative fuel can solve the problem of finding new oil fields, and also, due to the absence of emissions into the atmosphere, it can solve the problem of air pollution. Hydrogen also has the following properties that increase its competitiveness as an alternative fuel:

- Widespread availability of hydrogen [6];
- Converting hydrogen to electricity is fast and efficient;
- Hydrogen products and hydrogen itself, if leaked, do not harm the environment;
- Reduced emissivity of a hydrogen flame in comparison with a hydrocarbon flame [7-8];
- Heat transfer to the walls of the combustion chamber is less. This has a positive effect on the efficiency of a hydrogen engine [9-11].

2. Hydrogen technologies in engines (problem statement, calculation method, main results)

There are two main requirements that hydrogen must meet: burn quickly and completely. The factor to be taken into account in the design of the structure is the torque and the specific effective fuel consumption, which should be higher than that of gasoline-powered vehicles. For the conversion to hydrogen fuel, the well-known ZMZ-672-11 engine was chosen, with which PAZ buses were equipped. Engine specifications:

- Gasoline;
- Number of cylinders: 8;
- Power: 88.3 kW (120 hp);
- Rotation frequency: 3200 rpm;
- Torque: 284.5 N·m.

The thermodynamic calculation of the piston engine cycle was carried out according to the Grinivetsky-Masing method. Only the type of fuel (chemical composition) changed during the calculations, all other parameters of the engine cycle remained unchanged. Approximate data on the key parameters of the thermodynamic cycle and the technical and economic indicators of a piston engine can be obtained by calculating using this technique. It should be noted that the calculation results must be verified experimentally during bench tests. This is the goal of further research on this topic.

Thermodynamic calculations performed for this engine running on gasoline and hydrogen showed that the specific fuel consumption for hydrogen fuel is 20% less than that for a gasoline engine. The main indicators for comparison are listed in table 1.

Due to the fact that the combustion of the gasoline mixture in a gasoline engine is slower, fuel enters the combustion chamber before the piston reaches its top dead center. Since the gas in a hydrogen engine ignites instantly, it becomes possible to shift the injection time until the piston begins to return downward [12-13]. At the same time, for normal engine operation, a small pressure in the fuel system (up to 4 atmospheres) is sufficient. Under optimal conditions, the hydrogen motor is capable of operating with a closed-type feeding system. This means that atmospheric air is not used
during the formation of the mixture. After the end of the compression stroke, steam remains in the cylinder, which is directed to the radiator, condenses and becomes water. The implementation of this option is possible if an electrolyzer is mounted on the machine - a device that separates hydrogen from H$_2$O for subsequent reaction with O$_2$ [14-15].

Table 1. Comparative table of the main indicators of gasoline and hydrogen engines.

| Parameter                  | Value for gasoline | Value for hydrogen |
|----------------------------|--------------------|--------------------|
| Efficiency                 | 0.292              | 0.112              |
| Specific fuel consumption  | 0.272 g/kW·h       | 0.228 g/kW·h       |

To store hydrogen on board the bus, hydrogen tanks with a three-layer structure made of carbon fiber-reinforced plastic are used. They provide the necessary security and do not take up much space. Each tank is vacuum insulated and can be supplied vertically or horizontally.

Special installations are used to produce hydrogen. The principle of obtaining is the electrolysis of water. For this, a bipolar cell package is used. When current is applied to the stack of cells, hydrogen and oxygen are generated. The gases are then directed to a gas separator, which is a double stainless steel pressure vessel. Then hydrogen enters the purification system and is purified to a minimum level of 99.998%. The last stage occurs when the gas is cooled. Hydrogen and oxygen gases are cooled with previously cooled water. Further, there is filtration and removal from the gas stream.

Manufacturing hydrogen engines is also more environmentally friendly than manufacturing gasoline engines. As shown in table 2, the production of diesel engines uses up to 326.9 MJ of energy consumption. Energy consumption for hydrogen is 31% less.

Table 2. Comparative characteristics of pollutant emissions in the production of various types of fuel.

| Production type       | Petrol     | Hydrogen   |
|-----------------------|------------|------------|
| Total energy, MJ/100 km| 326.9      | 225.8      |
| Emissions, g/100 km   |            |            |
| CO$_2$                | 23.9       | 7.6        |
| Volatile organic matter| 33.2     | 16.6       |
| CO                    | 135.3      | 27.2       |
| Nitrogen oxides       | 22.8       | 11.0       |
| Solid particles ranging in size from 2.5 to 10 μm | 12.2 | 12.5 |
| Solid particles ranging in size less than 2.5 μm | 5.1 | 5.7 |
| Sulfur oxides         | 16.2       | 28.6       |

Comparing emissions from the production of two types of fuel, we can conclude that the share of emissions of harmful substances in the production of hydrogen is much less than in the production of gasoline. Accordingly, hydrogen engines have enormous potential [16-19].

3. The practical aspect of the use of hydrogen in transport

To assess the efficiency (profitability) of using hydrogen in engines, we calculated the payback of a bus route in the city of Ekaterinburg (Russia). The length of the round-trip route is 42 kilometers. There are 20 buses running on this route. Let's make calculations for the profit from the use of hydrogen fuel on this route. The average bus mileage per year is approximately 70,000 km. The fuel
consumption of the PAZ-3205 bus is 34 liters per 100 km. In Russia, the price of one liter of gasoline is 42.8 rubles. (as of January 6, 2021). The price of 1 liter of hydrogen is 38.4 rubles.

The amount of gasoline required to refuel one bus per year is:

\[ 34 \times 700 = 23,800 \text{ liters} \]  

(1)

The cost of refueling one bus per year is:

\[ 42.8 \times 23,800 = 1,018,640 \text{ rubles}. \]  

(2)

From the calculations made earlier, it follows that the consumption of hydrogen is 20% less than the consumption of gasoline. Therefore, the considered engine, when running on hydrogen, will consume 24 liters of hydrogen per 100 km. Accordingly, the amount of hydrogen required to refuel one bus per year is:

\[ 23,800 \times 0.8 = 19,040 \text{ liters} \]  

(3)

Thus, the cost of refueling one hydrogen bus per year is:

\[ 19,040 \times 38.4 = 731,136 \text{ rubles} \]  

(4)

The cost of gasoline fuel for twenty buses per year is:

\[ 1,018,640 \times 20 = 20,372,800 \text{ rubles (approximately 220,000 Euro)} \]  

(5)

The cost of hydrogen fuel for twenty buses per year is:

\[ 731,136 \times 20 = 14,622,720 \text{ rubles (approximately 159,000 Euro)} \]  

(6)

The annual benefit when using hydrogen fuel for the bus fleet (20 units) is 5,750,080 rubles (about 62,500 Euro).

According to expert estimates, the construction and commissioning of a hydrogen production plant will require approximately 46,180,505 rubles. Thus, the payback period of the plant will be about 8 years (46,180,505/5,750,080 ≈ 8).

### 4. Conclusions

The conducted research revealed that the specific fuel consumption for hydrogen is 0.228 g/kW·h, and for a gasoline engine – 0.272 g/kW·h. The effective efficiency index for a hydrogen engine is 0.112, for a gasoline engine – 0.292. It turns out that the fuel consumption on hydrogen fuel is 20% less than the consumption in a gasoline engine. The problem of increasing the efficiency of a hydrogen engine was not considered in this study.

The article presents a computational and analytical assessment of the efficiency of using hydrogen fuel in an engine in relation to the bus fleet of the city of Yekaterinburg. As a result, it was found that the payback period for the transfer of 20 buses to hydrogen is about 8 years.

It is also important to note that hydrogen can be obtained from a wide variety of domestic resources with the potential for near-zero greenhouse gas emissions.

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