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IMPROVEMENT OF ENERGY EFFICIENCY AND ENVIRONMENTAL SAFETY OF INTERNAL COMBUSTION ENGINES BY USING BINARY FUEL MIXTURES WITH HYDROGEN

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This paper addresses current issues related to improving the efficiency of fuel use in internal combustion engines and reducing the environmental impact of fuel combustion. It is demonstrated that incorporating hydrogen into mixtures with liquid fuels enhances the fuel's energy potential and combustion completeness. This approach aligns with the goals of sustainable development by reducing reliance on liquid hydrocarbon fuels and mitigating the harmful effects of pollutant emissions. The study proposes producing hydrogen via chemical reactions directly at the point of use, in quantities required for operation. These reactions enable the use of readily available, non-toxic materials for the targeted generation of hydrogen and its incorporation into fuel mixtures. Calculations show that the energy consumption for decomposing 1 kg of water using diesel and AI-92 gasoline is 12.9 MJ/kg and 13.2 MJ/kg, respectively.

Keywords: internal combustion engine, fuel mixtures, hydrogen, synthesis gas, nitrogen oxides.

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Introduction

Internal combustion engines (ICE), diesel, and petrol engines are the main types of engines in road and water transport, small aviation, and railways. The efforts to replace ICE with electric ones have faced the energy supply problem. The relevance of the issues of improving the economy and reducing the toxicity of ICE is undeniable. Hydrogen portion injection into the engine cylinders will improve combustion conditions, increase compression in the cylinders, and reduce liquid fuel consumption, as well as the content of toxic components in the exhaust gases by increasing the combustion temperature of the mixture.

One of the major trends of the late 20th and early 21st centuries is the continuing growth in the number of vehicles [1]. At the same time, sales of electric and hybrid vehicles are increasing (Fig. 1), reflecting a global trend towards sustainable transport.

Tightening environmental regulations [3] led to a steady increase in the complexity of design solutions in the ICE: additional external systems, such as catalytic converters, which burn off toxic components contained in the exhaust gases; exhaust gas recirculation (EGR) systems; systems of chemical neutralization of nitrogen oxides by injecting urea; installation of filter-catalysts to reduce the toxicity of exhaust gases, etc. Considering these developments, the toxicity of exhaust gases should not exceed the currently established Euro 6d standards (Table 1).

Fuel combustion in internal combustion engine cylinders takes place over a very short time with variable volume and pressure and uneven distribution of liquid fuel microdroplets across the volume of the combustion chamber. A specific issue is the size of the fuel droplets forming the fuel suspension; the smaller the droplet size, the higher their oxidation

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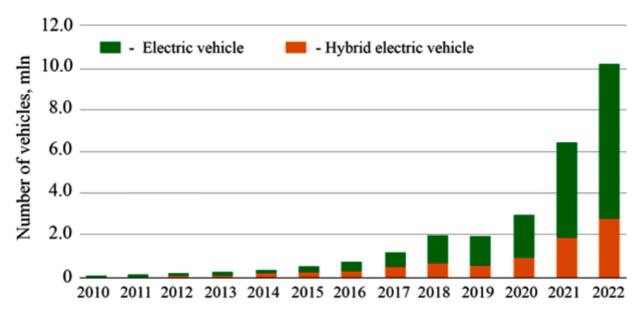


Fig. 1. The trend toward increasing sales of electric and hybrid electric vehicles [2]

European emission standards Euro 6d, g/km*

Table 1

For passenger cars (Category M)												
Engine's type	CO	THC	VOC	NOx HC+NOx		P	PN, g/kWh					
Diesel	0.500	_	_	0.080	80 0.170 0.0045		6.10^{11}					
Petrol (Gasoline)	1.000	0.1000	0.068	0.060	_	0.0045	0.0045 6.10^{11}					
For light commercial vehicles with reference weight ≤1305 kg (Category N1, class I),												
Engine's type	CO	THC	NMHC	NOx	HC+NOx	PM	PN, g/kWh					
Diesel	0.500	_	_	0.080	0.170	0.0045	6.10^{11}					
Petrol (Gasoline)	1.000	0.1000	0.068	0.060	_	0.0045	6.10^{11}					
For light commercial vehicles 1305-1760 kg, reference weight (Category N1, class II)												
Diesel	0.630	_	_	0.105	0.195	0.0045	6.10^{11}					
Petrol (Gasoline)	1.810	0.130	0.090	0.075	_	0.0045	6.10^{11}					
For light commercial vehicles >1760 kg reference weight max. 3500 kg (Category N1, class III and N ₂)												
Diesel	0.740	_	_	0.125	0.215	0.0045	6.10^{11}					
Petrol (Gasoline)	2.270	0.160	0.108	0.082	_	0.0045	6.10^{11}					
For heavy diesel engines, g/kWh												
Test cycle	CO	HC	Smoke, m ⁻¹	NOx	NH ₃ , ppm	PM	PN, g/kWh					
WHSC	1.5	0.13	_	0.4	10	0.01	8.10^{11}					
WHTC	4.0	0.16	_	0.46	10	0.01	6.10^{11}					

Note: * – THC is the general forms are total hydrocarbons; NMHC is nonmethane hydrocarbons; NMOG is nonmethane organic gas; VOC is volatile organic compounds; HC is hydrocarbon; and P, PM, PN are particulate matters.

surface and, consequently, the combustion efficiency [4].

Improvement of the combustion efficiency of liquid fuels can be been achieved in several different ways:

- ensuring a stable microdroplet size by changing the design of the injection nozzle;
- providing conditions for efficient vaporization of large fuel droplets and their transformation into the smallest droplets, as well as mixing with air in

the cylinder;

— using forechambers and grids (so-called forechamber engines), when the basic volume of fuel is injected into the cylinder, and a small portion into a special forechamber, where a saturated mixture is created, which is ignited by a candle and bursting out from the forechamber flame ignites the rest of the mixture.

In fact, the inability to provide ideal conditions for fuel combustion in a wide range of varying loads

led to «dieselgate», when the car's electronic control system, having diagnosed the dynamics of the car's movement as defined by the test regulations, switched the operation of the diesel engine to the lowest emission mode, to the detriment of its efficiency and power. Obviously, in real mode, when the car maneuvers in the traffic flow, moving along the highway with continuously changing speed, road surface quality, slopes, and the vehicle's weight, it is almost impossible to achieve maximum fuel combustion. Furthermore, it is challenging to meet the requirements of the standards, even for the most modern designs¹. Everything mentioned above is also applicable to gasoline engines with spark ignition.

Environmental requirements for ICE are thus in conflict with technical and economic ones. At the same time, the steady growth of motor fuel prices leads to the need to minimize fuel consumption.

Nowadays, the electric vehicle sector is developing dynamically, mainly due to the policy of providing tax benefits and, subsidies and other preferences to their owners. However, the proportion of electric vehicles in the total number of vehicles is still low. At the same time, the biggest parts of electric vehicles are passenger cars, city buses and light commercial trucks. The challenges to complete substitution are well known: limited mileage of electric vehicles from a single charging cycle insufficiently developed charging infrastructure, battery mass characteristics, and lifecycle, charging time, external temperature effects, as well as problems with production and utilization of spent batteries [5–9].

One of the options for eliminating the disadvantages of electric cars is fuel cell vehicles [10]. Hybrid vehicles are mainly cars and buses, representing a transition model from fully petrol (diesel) to electric vehicles.

The aim of the work is to reduce dependence on liquid hydrocarbon fuels, their consumption, and the toxicity of the exhaust gases by using binary fuels with hydrogen content. It is proposed to use binary fuels diesel/hydrogen and petrol/hydrogen. Moreover, hydrogen will be produced at the point of use by chemical reaction in volumes that will be directly consumed by the engine.

One of the options for reducing the toxicity of exhaust gases and improving the efficiency of engines is the use of alternative fuels (Table 2).

Hydrogen is the most energy-intensive and environmentally friendly fuel. Hydrogen can be produced from various sources, such as water, fossil fuels, and biomass. Hydrogen has the highest calorific value per weight unit among all conventional fuel sources and low energy content per volume unit. Therefore, hydrogen can be effectively used as a substitute for conventional fuel sources [11,12].

Fuel cell vehicles can use hydrogen, retaining all the advantages of traditional engines («perfect» traction, high dynamics, and engine overload capacity) with high energy efficiency and fast charging capability. Several leading European, American, and Chinese manufacturers have launched models of cars, light vans, and buses with fuel cells. Still, their total number is insignificant compared to battery electric vehicles. The main reason is difficulties with the safe storage of hydrogen.

Compressed hydrogen storage (e.g., Toyota Mirai) requires high-strength multi-layer steel cylinders with austenitic steel inner liners (ratio of approximately 33 kg of steel per 1 kg of hydrogen). The service life of such cylinders is short. The ability of hydrogen to diffuse through a carbon alloy (e.g., steel) is sometimes accompanied by its destruction due to hydrogen-carbon interaction. Hydrogen corrosion of the metal leads to leaks, creating the risk of a gas explosion. Composite and carbon fiber cylinders are not free from such disadvantages due to the permeability of their walls to hydrogen [13]. None of the current hydrogen storage methods allow for safe and economical hydrogen storage on vehicles.

Results and discussion

Since the vast majority of vehicles, mobile machinery, and mechanisms are equipped with internal combustion engines, the most rational option would

Energy intensity of motor fuels

Table 2

Fuel type	hydrogen (gas)	natural gas (methane)	petroleum gas (propane- butane)	gasoline (AI-92)	diesel fuel	methanol	dimethyl ether
Specific heat of combustion, weight unit, MJ/kg	141	45	43.8	44	43	22.7	30.0

¹ IEA HEV Task 35 – The State of Art on Fuel Cell Vehicle and Technology. Chief Editor: Ock Taeck Lim. Final Report, June 28. – 2022. https://ieahev.org/wp-content/uploads/2023/05/Task-35-_final-report-2022-0627.pdf.

be to convert them to run on diesel/hydrogen and petrol/hydrogen binary fuels. At the same time, the underdeveloped hydrogen-charging infrastructure and the issues of cost-effective and safe hydrogen storage can be avoided by creating compact on-vehicle hydrogen generators. Hydrogen will be produced in volumes immediately consumed by the engine, taking into account changes in its operating modes, thus minimizing the possibility of losses.

Hydrogen can be produced chemically on the vehicle using acetylene-type generators or Kipp's apparatus.

The following most promising reactions can be used:

1. Action of alkalis on zinc or aluminum:

2Al+6NaOH+6H₂O
$$\rightarrow$$
2Na₃[Al(OH)₆]+3H₂ \uparrow , (1)

$$Zn+2KOH+2H_2O \rightarrow K_2[Zn(OH)_4]+H_2\uparrow$$
. (2)

2. Reaction of sodium borohydride with water:

$$NaBH_4 + 2H_2O \rightarrow NaBO_2 + 4H_2 \uparrow.$$
 (3)

The use of sodium borohydride allows for the generation of significant amounts of hydrogen at relatively low energy consumption.

3. Reaction of aluminum with water in the presence of gallium as a catalyst that destroys the oxide film on the metal surface:

$$2A1+6H_2O=2A1(OH)_3+3H_2\uparrow$$
. (4)

The latter method of hydrogen production is the most promising since it is based on the use of chemically non-active and non-toxic (aluminum, water) and low-toxic (gallium) components. The reaction takes place at low temperatures with high speed and efficiency.

Technically, the creation of this kind of generator is not difficult. It is possible to transport gallium-doped aluminum in the form of granules by a screw feeder of controlled capacity or in the form of a belt pulled by a special device into a reservoir with water. Since the reaction of aluminum with water is reversible, aluminum hydroxide can be reduced to pure aluminum. Gallium is not consumed in the reaction.

Since the flashing of the gas-air mixture is realized by the injection of a small portion of diesel fuel, modifications to the diesel engine are minimized. The flash point of the hydrogen/diesel mixture is lower than that of pure hydrogen and does not require special alloys.

A gasoline engine can theoretically use pure hydrogen; however, in this mode, there are a number of issues with thermal and dynamic loads on the engine. Therefore, it is more appropriate to use a binary hydrogen and gasoline fuel.

Hydrogen to power the engine can be obtained from a compact electrolyzer located in the engine compartment of the vehicle. The engine-mounted generator that powers the electrolyzer allows the hydrogen production to be flexibly varied to reflect changes in engine operation.

The method of producing hydrogen, and in fact, hydrogen-oxygen mixture also known as Brown's gas, water gas, brown gas, hydrogen, dihydrogen, green gas, Klein gas, oxyhydrogen, is already well practiced.

During electrolysis of aqueous solutions of alkalis or acids, hydrogen is released at the cathode, for example:

$$2H_3O^+ + 2e^- \rightarrow H_2\uparrow + 2H_2O. \tag{5}$$

The production of compact electrolyzers for injector and diesel vehicles is already well developed.

The methodology for calculating the energy feasibility of using hydrogen as a fuel component is presented below.

1. Determination of energy consumption for water electrolysis.

During the reaction, hydrogen is burned with heat release of 285.2 kJ/mol (with liquid water as a final product). The most advanced electrolyzers produce efficiencies of up to 85%, i.e., the consumption for water electrolysis is 285.8/0.85=336 kJ/mol.

2. Conversion of energy from value «mole» to kilogram.

Since the molar mass of water is 18 g/mol, to convert from energy per mole to energy per kilogram, multiply the value in kJ/mol by the coefficient (1000 g/18 g):

 $336 \text{ kJ/mol} \cdot (1000/18) = 18666 \text{ kJ/kg}.$

3. Conversion from energy in kJ into power in kWh.

The energy required to decompose 1 kg of water can be converted at 1 kWh=3600 kJ: 18666 kJ/3600=5.19 kWh.

Thus, to decompose 1 kg of water into hydrogen and oxygen, 5.2 kWh or 18666 kJ is required.

However, a part of the diesel consumed by the engine must be used to decompose water into hydrogen and oxygen.

4. Calculation of diesel fuel consumption to provide the required energy.

The calorific value of diesel fuel is 43 MJ/kg, but considering the efficiency of the diesel engine (approximately 30%), the useful amount of energy is 43 MJ/kg·0.3=12.9 MJ/kg.

To provide the 18666 kJ needed to electrolyze 1 kg of water requires X=18.666 MJ/12.9 MJ/kg=1.45 kg of diesel.

5. Conversion of diesel mass to volume.

When the density of diesel is 0.83 g/cm³ (i.e., 0.83 kg/L), the volume corresponding to 1.45 kg of diesel is defined as

V=1.45 kg/0.83 kg/L=1.75 L.

This is the diesel flow rate required to decompose 1 kg of water.

6. Determination of amount of energy produced when hydrogen is burned.

After electrolysis, hydrogen burns, turning into water in the form of vapor. The heat of formation of water (in the vapor state) is 242 kJ/mol. Converting this value into MJ/kg is as follows:

242 kJ/mol·(1000/18)=13.44 MJ/kg.

7. Calculation of energy benefit.

The energy benefit is defined as the difference between the heat of water formation and the useful energy from diesel fuel:

13.44 MJ/kg-12.9 MJ/kg=0.54 MJ/kg.

The advantages of synthesizing gas as a fuel are associated with free hydrogen and oxygen in it.

The addition of a hydrogen-oxygen mixture completely and uniformly occupies the entire volume of the combustion chamber in contrast to the plume of microdroplets in injected liquid fuel. This will increase the speed of spreading of the ignition front, as well as the flash energy and the completeness of liquid fuel combustion due to the growth of temperature in the cylinders and the presence of an additional portion of oxidant. This would increase the indicator efficiency. Adding even 10% of synthesis gas leads to a 30–40% reduction in diesel fuel consumption.

More significant than increasing efficiency and reducing diesel consumption for vehicles and autonomous machines and mechanisms is the reduction of exhaust emissions. When 10% of hydrogen is added, the content of such a strong carcinogen as soot in the exhaust gases is reduced by 75%. As the proportion of diesel fuel injected into the cylinder decreases, benzopyrene CO, CO₂, hydrocarbons, aldehydes, and benzopyrene emissions

also decrease significantly. However, an increase in the specific weight of hydrogen in the fuel mixture leads to an increase in the mixture combustion temperature and detonation rate. This has a number of negative consequences: increased nitrogen oxide emissions; increased load on the cooling system and the engine cylinder-piston group, leading to higher wear.

The increase in nitrogen oxides can be easily neutralized by applying the effective urea injection technology into the engine exhaust system. Urea (NH_2CONH_2) reacts with nitrogen oxides (NO_x) present in emissions, primarily nitrogen oxides (NO) and nitrogen dioxide (NO_2) . As a result, nitrogen (N_2) and water vapor (H_2O) are produced by the reaction:

$$NH_2CONH_2+2NO (or NO_2)+$$

 $+1/2O_2=2N_2+CO_2+2H_2O.$ (6)

At 50% replacement of diesel fuel with hydrogen, engine rough running increases by more than 100% and cylinder pressure by 30%. The consequence of increased dynamic loads is reduced engine service, increased maintenance, and repair costs. Therefore, for the operating conditions of a particular engine it is necessary to select a rational ratio in the fuel mixture of diesel and hydrogen, providing proper operating modes of the engine.

Similar calculations carried out for a gasoline engine show that with the calorific value of 44 MJ/kg for gasoline grade AI-92 and the efficiency of the gasoline engine at 30%, the useful amount of energy is 44·0.3=13.2 MJ/kg. Then the amount of gasoline AI-92 for decomposition of 1 kg of water will be: X=18.666/13.2=1.41 kg. At a density of gasoline of 0.74 g/cm³, the volume is V=1.41/0.74=1.9 L. Consequently, the energy benefit would be 13.44–13.2=0.24 MJ/kg. However, the main advantage is achieved by improving the combustion conditions of gasoline, increasing its completeness, and reducing the toxicity of exhaust gases, which is much more relevant for a petrol engine, which releases more toxic components than for a diesel engine.

Conclusions

The conducted analyses and calculations to improve energy efficiency and environmental impact of internal combustion engines using binary fuel mixtures with hydrogen allow concluding the following points:

1) Using synthesis gas generators will reduce emissions and fuel consumption of vehicles and machinery with ICE, renewing both the existing and newly commissioned fleet of vehicles.

- 2) It is necessary to determine the optimum ratio of hydrogen in the binary mixture for each specific type of engine to preserve engine service.
- 3) The energy consumption of diesel and AI-92 gasoline in the decomposition of 1 kg of water is at about the same level, 12.9 MJ/kg and 13.2 MJ/kg, respectively.
- 4) Applying synthesis gas on petrol engine vehicles may allow the use of lower octane petrols.

Additionally, the proposed approach has the following advantages:

- 1) Direct production of hydrogen at the point of consumption, which eliminates the need for hydrogen storage and transportation and reduces risks and investment costs.
- 2) Flexible hydrogen supply control allows quickly adapting the amount of hydrogen produced to the current engine load.
- 3) Improving the combustion process by evenly distributing hydrogen in the fuel mixture, which increases thermodynamic efficiency and reduces emissions.
- 4) The use of advanced materials and catalysts (e.g. gallium), which reduces energy costs and ensures process stability at low temperatures.

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ПІДВИЩЕННЯ ЕНЕРГОЕФЕКТИВНОСТІ ТА ЕКОЛОГІЧНОЇ БЕЗПЕКИ ДВИГУНІВ ВНУТРІШНЬОГО ЗГОРЯННЯ ЗА РАХУНОК ВИКОРИСТАННЯ БІНАРНИХ ПАЛИВНИХ СУМІШЕЙ З ВОДНЕМ

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У роботі розглянуто актуальні питання розвитку ефективності використання палив для двигунів внутрішнього згоряння, а також зниження негативного впливу спалювання палива на навколишнє середовище. Показано, що використання водню в суміші з рідким паливом дає змогу підвищити енергетичний потенціал палива та повноту згоряння, що відповідає завданням сталого розвитку щодо зменшення залежності від рідких вуглеводневих палив і негативного впливу шкідливих викидів. Пропонується одержувати водень шляхом хімічних реакцій безпосередньо на місці споживання в необхідних обсягах. Хімічні реакції дозволять використовувати доступні нетоксичні матеріали для цілеспрямованого виробництва водню та його використання в паливних сумішах. Розраховано, що енерговитрати дизеля та бензину АІ-92 на розкладання 1 кг води становлять 12,9 МДж/кг та 13,2 МДж/кг, відповідно.

Ключові слова: двигун внутрішнього згоряння, повна суміш, водень, синтетичний газ, оксиди азоту.

IMPROVEMENT OF ENERGY EFFICIENCY AND ENVIRONMENTAL SAFETY OF INTERNAL COMBUSTION ENGINES BY USING BINARY FUEL MIXTURES WITH HYDROGEN

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This paper addresses current issues related to improving the efficiency of fuel use in internal combustion engines and reducing the environmental impact of fuel combustion. It is demonstrated that incorporating hydrogen into mixtures with liquid fuels enhances the fuel's energy potential and combustion completeness. This approach aligns with the goals of sustainable development by reducing reliance on liquid hydrocarbon fuels and mitigating the harmful effects of pollutant emissions. The study proposes producing hydrogen via chemical reactions directly at the point of use, in quantities required for operation. These reactions enable the use of readily available, non-toxic materials for the targeted generation of hydrogen and its incorporation into fuel mixtures. Calculations show that the energy consumption for decomposing 1 kg of water using diesel and AI-92 gasoline is 12.9 MJ/kg and 13.2 MJ/kg, respectively.

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