Reducing the Level of Nitrogen Oxides in Exhaust Gases of a High-Speed Hydrogen-Powered Diesel Engine

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***Abstract*—The relevance of the widespread introduction of hydrogen as fuel for the transport and stationary engines is obvious. The proposed paper describes the working process of a still little studied hydrogen-powered diesel engine with direct injection of hydrogen gas. The study was carried out using a 3D mathematical model based on the fundamental equations of the Navier-Stokes type, which were solved by the numerical method of control volumes using the CRFD code AVL FIRE. Numerical experiments have shown that with an increase in the amount of hydrogen injected into the cylinder at a constant value of the excess air ratio, the quantities of nitrogen oxides generated in the combustion chamber can increase. An explanation is given for the reason for this phenomenon, which is not characteristic of the traditional diesel engines. It was found that by changing the regulating (moment of hydrogen injection) and design (shape of the combustion chamber, diameter and number of nozzle holes) parameters, it is possible to achieve a significant reduction in the emission of nitrogen oxides. The values of these parameters, contributing to a significant reduction in the emission of nitrogen oxides, have been determined.**

Keywords—hydrogen-powered diesel engine; 3D modeling; shape of the combustion chamber; nozzle design.

I. Introduction

The widespread use of hydrogen, as an alternative to petroleum-derived traditional fuels in transport and stationary energy production, is the way forward for solving environmental and energy-related problems. The main advantages of using hydrogen as a motor fuel lie in its remarkable thermophysical properties, such as high values of the heat of combustion, flame propagation velocity, the minimum ignition energy, a wide range of inflammability in terms of the excess air factor, as well as in complete decarbonization of exhaust gases. The only harmful component of the latter are nitrogen oxides NOx, the reduction of which by controlling the injection moment (ignition dwell angle) and changes in the shape of the combustion chamber, as well as the design of the nozzle, and this is what this paper focuses to.

All of the research completed so far has been mostly on the hydrogen engines with carburation and positive ignition. The hydrogen-powered diesel engine with direct injection of the gas hydrogen into the cylinder has obvious advantages, both from an environmental point of view (NOx emissions) and in terms of fuel efficiency (engine efficiency). Despite this, the first incisive pilot studies proving the long-term benefits of developing the hydrogen-powered diesel engine were conducted by H. Rottengruber and others at the Technical University of Munich [1, 2]. Later, it's where the pilot studies were conducted on the ignition delay of various hydrogen-containing fuels [3]. On the basis of the experimental data obtained, the 3D mathematical models were developed [4, 5, 6], allowing to monitor the change in the local parameters of the working fluid in the cylinder, which determine the environmental performance of the engine, which is in turn very difficult and time-consuming, and sometimes impossible in the process of a pilot study. It should also be noted that recently the problem of developing the hydrogen-powered diesel engine has become even more urgent in connection with the desire to drastically reduce CO_2 emissions [7, 8, 9]. Let us emphasize that the question of the influence of a number of design parameters on the combustion process and the formation of nitrogen oxides in the hydrogen-powered diesel engine has not been practically studied using the mathematical modeling methods.

The proposed study is aimed at 3D modeling of the working process of the hydrogen-powered engine and the generation process of nitrogen oxides, as well as the determination of those values of regulated and design parameters of the engine that can reduce the emissions nitrogen oxides.

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II. A BRIEF DESCRIPTIN OF THE ENGINE UNDER STUDY AND A 3D MATHEMATICAL MODEL OF THE WORKING PROCESS

The object of investigation was a high-speed hydrogen-powered diesel engine, which is a hydrogen-converted modification of the base four-stroke, V-shaped, 24-valve water-cooled diesel engine with the following technical data: number of cylinders i=6; cylinder diameter/piston stroke D/S=130/140 mm/mm; compression ratio ε=16,5; effective power Ne=315 kW; crankshaft speed n=2000 min^{-1}, the combustion chamber shape of YaMZ type.

The mathematical model is based on the fundamental equations of conservation of momentum (Navier-Stokes equations), energy (Fourier-Kirchhoff equations), diffusion (Fick equation) and continuity, describing unsteady three-dimensional turbulent motion in the gas exchange systems and in the cylinder of the hydrogen-powered diesel engine. After averaging with respect to Favre, these equations are written in the Reynolds form and supplemented by the equations of the k-f-ζ model of turbulence. The combustion process is simulated using the Magnussen-Hjertager model, and the generation process of nitrogen oxide is based on the extended Zeldovich mechanism. For a numerical solution, the semi-implicit method SIMPLER (Semi-Implicit Method for Pressure-Linked Equations-Revised) is used, which was designed for a step-by-step calculation of the "predictor-corrector" type. Numerical experiments were carried out using the 3D CRFD code AVL FIRE. A detailed description and analysis of these equations, models and methods of solution are published in [4, 5, 6, 10, 11].

When converting the traditional serial diesel engines running on the hydrocarbon diesel fuel to hydrogen, a comparative analysis of the processes occurring in the combustion chambers of the base diesel and the hydrogen-converted diesel engines was carried out under conditions formulated in [6]: 1) Identity of the main dimensions D and S, as well as ε and the shape of the combustion chamber; 2) Identity of the available amount of heat entering the combustion chamber with the inject fuel. The latter condition is satisfied on the basis of the ratio of the mass cyclic hydrogen inlets and the diesel fuel [6]. It was shown that under these conditions in the combustion chamber of the hydrogen-powered diesel engine, the local temperatures have relatively high (compared to the base diesel engine) values and lead to increased (by about ~ 10%) values of the total mass amount of nitrogen oxides per cycle.

Reducing the level of nitrogen oxides in the exhaust gases of the hydrogen-powered diesel engine would be achieved through the successful selection of regulating (the hydrogen injection timing angle) and designing (CC shape, number of nozzle openings in the injection nozzle) parameters.

III. THE INFLENCS OF THE HYDROGEN INJECTION TIMING ANGEL (HITA)

The HITA defines the moment of fuel injection and, obviously, its value significantly affects the efficient and environmental performance of the engine [3]. The flame propagation velocity during the combustion of the stoichiometric mixtures with air in the case of hydrogen is approximately 5-6 times higher than in the case of a diesel fuel, gasoline or natural gas [12]. In this regard, small changes in the hydrogen gas emission ratio can affect the course of the combustion and NOx generation. The modeling of the generation process of NOx, carried out when changing the HITA by 1^0 of crankshaft degree, showed a significant effect of the moment of direct injection of hydrogen into the cylinder. This is confirmed by the results obtained for three different values of the HITA – 7^0, 6^0 and 5^0 of crankshaft degree (or the corresponding injection moments $\varphi_{inj} = 353^0$, 354^0 and 355^0 of crankshaft degree (Fig. 1). Note that the quantities of nitrogen oxides indicated in Figure 3 in the cylinder of the hydrogen-powered diesel engine correspond to the moment of opening of the exhaust valves, that is, these are the total concentrations in the cylinder for the working cycle. In the investigated range of variation of φ_{inj}, a decrease in the injection lead angle by 1^0 of crankshaft degree leads to a decrease in the total amount of nitrogen oxides per cycle by about 7-8%.

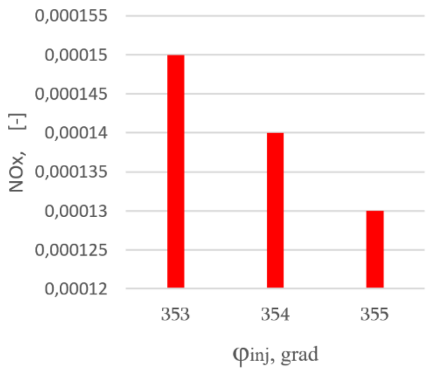


Fig.1. *Total nitrogen content per working cycle (mass portion), depending on the moment of hydrogen injection φ_{inj}.*

However, this process is accompanied by a decrease in the maximum cycle pressure pz and a deterioration in the effective performance of the working process.

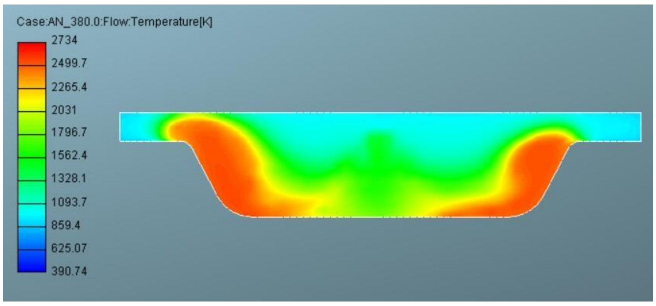
Modeling the change in the local temperatures of the working fluid in the combustion chamber, depending on the moment of hydrogen injection, demonstrated that with a relatively large injection lead angle (that is, with early injection, when φ_{inj} = 353°), the first sources in the combustion chamber manage to form already by the time when the piston is in the position of top dead centre (TDC), and with relatively late injection (φinj = 355°), these sources are not so visible. Note that the intensity of local generation of nitrogen oxides depends on the intensity of the growth of local temperatures and, obviously, it changes in a similar way depending on the moment of hydrogen injection. In addition, with early injection, the rate of pressure rise dp/dφ increases, which is caused by a sharper increase in the rate of heat generation at the initial stage of combustion, and, accordingly, the noise level increases when operating the engine.

Such different developments of the combustion processes depending on φinj leads to the fact that with early injection (φinj = 353°), the maximum values of the heat release rate (dQx/dφ)max, pressure pz and temperature Tz are higher, and their corresponding crankshaft degrees φ are closer to TDC (φ = 360°) than with late injection (φinj = 355°). This explains the fact that a decrease in NOx concentration with a later injection (Figure 1) can lead to a decrease in the efficiency of the cycle.

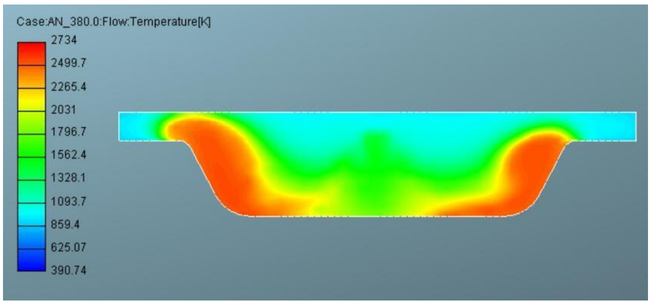
IV. THE INFLUENCE OF THE SHAPE OF THE COMBUSTION CHAMBER

When converting the serial compression-ignition diesel engines to the positive-ignition gas engine in order to prevent knocking, the compression ratio needs to be reduced. It is usually achieved through changing the shape and size of the combustion engine located in the piston. In the hydrogen-powered compression-ignition diesel engine, compared to a serial base diesel engine, higher compression ratio may be required, which is due to a higher autoignition temperature of hydrogen (585°C under atmospheric conditions) compared to a diesel fuel (250°C under the same conditions) [12]. In any case, the transition from the liquid to gaseous fuel is often associated with change in the compression ratio associated in turn with change in geometry of the combustion chamber.

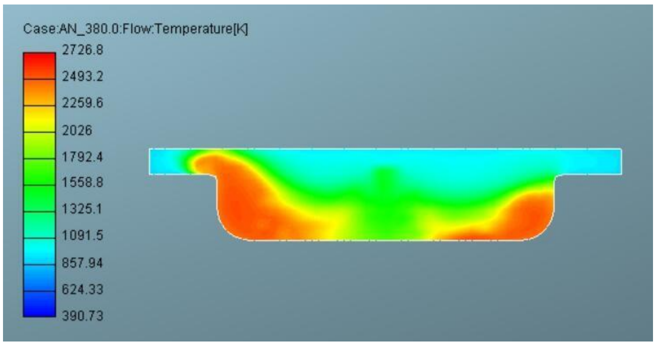
The invalidity of the prevailing opinion that in the gas-powered engines with spark ignition it is important to provide the compression ratio required for knock-free operation, and the shape of the combustion chamber is immaterial, was proved in [13]. The results of the numerical experiments carried out for the three different shapes of the combustion chamber of the hydrogen-powered diesel engine show a noticeable influence of the shape of the combustion chamber on change in the local temperatures of the working fluid (Figure 2).



a



b



c

Fig.2. *The instant temperature fields of working fluid in the volume of the combustion chamber depending on its shape, at crankshaft degree is φ=3800 : a – base combustion chamber (CC) of YaMZ type; b – conical (asymmetrical) CC; c – cylindrical (symmetrical) CC.*

We can see that in the cylindrical combustion chamber, when φ = 380° of crankshaft degree are the high-temperature zones, that is, the zones with intensive combustion occupy significantly less volume of the combustion chamber than in the conical or the base combustion chamber. It is obvious that the base combustion chamber of the YaMZ type, which is w-shaped (Figure 3), further contributes to an increase in the kinetic energy of turbulence (KET) of the working fluid in the cylinder, especially when the piston approaches the TDC, that is, to the moments of hydrogen injection and the start of ignition. This causes the effect of KET on the rate of heat release, depending on the shape of the combustion chamber, which has the appearance shown in Figure 3. As you can see, in the case of a base (w-shaped, YaMZ type) combustion chamber, the heat release rate is not only higher, but also its maximum instantaneous magnitude is closer to TDC (φ=360° of crankshaft degree, Figure 3) than in the case of the conical or cylindrical combustion chamber.

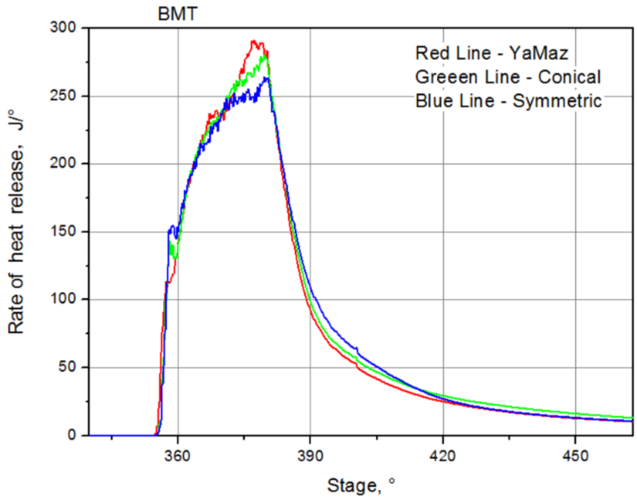


Fig. 3. *Change of rate of heat release (J/0crankshaft degree) in the cylinder of the hydrogen powered diesel engine depending on the shape of the combustion degree.*

It is obvious that the cycle maximum pressure p_z and its correspondence maximum value of the temperature T_z of the cylinder averaged by volume, as well as the total cyclic concentrations (mass portion) of nitrogen oxides in the case of a base combustion chamber is higher compared to the cylindrical and conical combustion chambers (Figure 4). Thus, the base combustion chamber, giving the best effective indicators of the cycle among the three study shapes of the combustion chamber, in terms of the emission of nitrogen oxides, remains below according to the meaning of nitrogen oxide is established (but not too far, see Figure 5) the other combustion chambers.

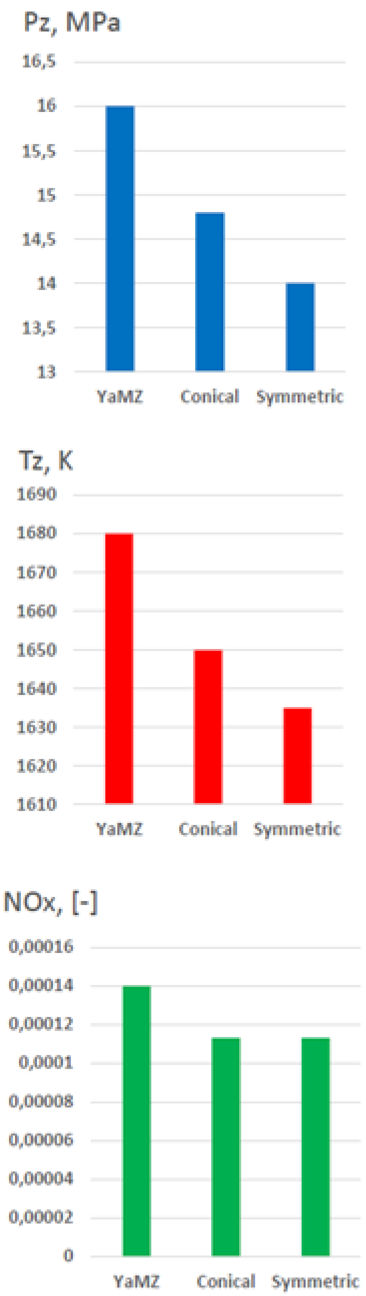


Fig. 4. *The influence of the shape of the combustion chamber on maximum pressure p_z and the temperature T_z averaged in terms of volume of the cylinder, and the total cycle concentration (mass portion) of nitrogen oxides NOx.*

Note that the reduction in NOx emissions in the hydrogen-powered diesel engine could be reduced significantly with the help of the exhaust gas recirculation methods proven in the traditional diesel engines [14], or by means of the homogenization of the combustion process in the diesel engine. The latter could be carried out, for example, by increasing the number of nozzle holes in the nozzle [15].

V.THE INFLUENCE OF THE NOZZLE DESING

The results of a pilot study, given in [12], demonstrate that the nozzle design, specifically the number and diameters of nozzle holes, can have a significant impact on the process of nitrogen oxide generation. In this work, the task is solved with the help of 3D CRFD programs AVL FIRE [11], allowing the turbulent combustion of hydrogen in the cylinder of the engine. Figure 5 illustrates the instant temperature fields and concentrations (mass portions) of nitrogen oxides in cylinder capacity.

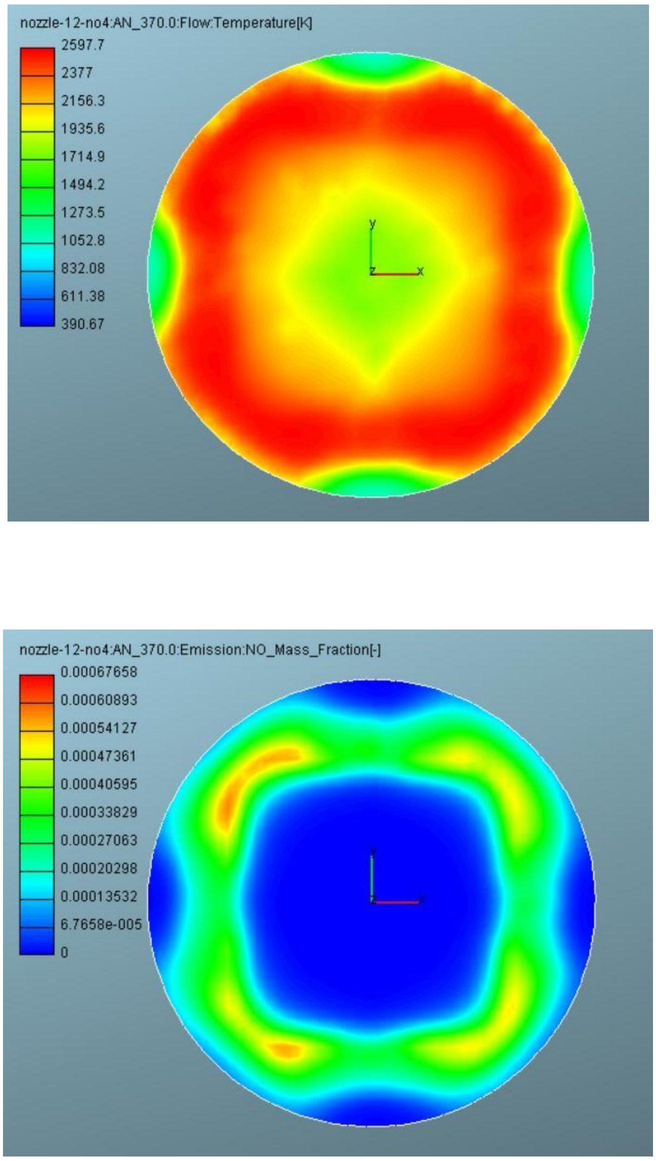
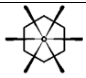
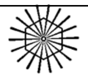


Fig. 5. *Instant values of the local temperatures and concentration (mass portion) of NOx in the combustion chamber of the hydrogen-powered combustion engine with a nozzle №2 (z=18, dc=0,42 mm, see Table 1), when crankshaft degree is φ=370°.*

The schemes of the nozzles under study, their geometrical parameters, as well as the cyclic values of the total quantities (mass portions) of nitrogen oxides, depending on the design of the nozzle end of the nozzle burner, are presented in Table 1.

TABLE I.

№	Nozzle diagram	Number of nozzles Holes, z	Diameters of nozzle holes, dc, mm	Total open flow area of holes, ΣF, mm^2	share of NOx (total mass portion per cyle)
1		6	0,24	0,27	0,0012
2		18	0,17	0,41	0,00022

As the number of nozzle holes increases, there occurs homogenization of the hydrogen-air mixtures, in which the flame from the first combustion sources spreads rapidly to the adjacent zone in cylinder capacity and covers more rapidly the volume of the combustion chamber (Figure 5). The rapid growth of heat release rate in the initial phase leads to an increase in pressure rise rate, which in turn contributes to increasing noise of the hydrogen-powered diesel engine. With other factors, the homogenization of mixtures leads to the regulation of local temperatures in the upper zones (Fig. 5) and lowering of the temperature cycle as a whole, and particularly the local temperatures themselves, which reflects the total cyclic concentration of nitrogen oxides (see Table 1).

VI. CONCLUSIONS

Numerical experiments performed during modeling of intra0cylinder processes of the traditional (base) and hydrogen-powered diesel processes showed significant difference between the natures of the conduct of these processes n the traditional and hydrogen-powered diesel engines during the injection and combustion of fluid diesel fuel. In the case of a diesel fuel, the processes of evaporation and carburation begin and occur on the outer surface of the injected fuel spray, where the first combustion sources appear. Hydrogen is more rapidly mixed with air by volume of the combustion chamber and ignites faster, the flame rapidly spreads to the volume of the combustion chamber.

An increase in the cyclic hydrogen consumption, when the aggregate excess air ratio remains constant, increases the mass of the hydrogen-air mixture in the cylinder and leads to higher density of working fluid. Provided that hydrogen injection pressure, limited by critical value, leading to a constant magnitude of hydrogen discharge through the nozzle, remains constant, hydrogen throw (the depth of penetration into the cylinder decreases). Hydrogen will accumulate near the nozzle, and due to lack of oxygen in this zone, the combustion process can be stretched out. This leads to a decrease in local temperature in the combustion chamber, and as a result, to an increase in local NOx concentrations. This phenomenon, earlier noted in the pilot studies on the hydrogen-powered diesel engines, conducted by H. Rottengruber and others [1, 2], has no place in the traditional diesel engines.

By changing the moment of hydrogen injection (injection timing angle φinj), it is possible to increase the effective performance of the hydrogen-powered diesel engine so that an increase in nitrogen oxides remains relatively small. In this regard, the value φinj = 353° should be taken as optimal for the investigated hydrogen-powered diesel engine. The conical combustion chamber from an environmental point of view has an advantage over the base chamber of the YaMZ type (reduces the emission of nitrogen oxides by about 15-18%) and leads to practically the same results as the cylindrical (symmetrical) chamber. As a result, it is recommended to choose the conical chamber, which, however, in terms of effective performance is not much inferior to the YaMZ-type chamber, but surpasses the symmetrical (cylindrical) chamber. According to the results of the study of two different designs of the nozzle end, it was found that the nozzle with an increased number of nozzle holes (18x0,17 mm) significantly reduces the emission of nitrogen oxides, does not significantly decrease the effective performance, and its use is advisable.

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