Influence of the exhaust gas recirculation on formation of NO\textsubscript{x} in the hydrogen engine working on the leaked mixture (Experiment and 3D modeling)

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Summary. Nitric oxides are the only components from the harmful ones limited by the legislation found in the exhaust gases of the hydrogen engine. For the purpose of their minimization and prevention of the anomaly burning processes as well (detonation combustion, early ignition, back fire), the use of the leaked hydrogen-air mixture is offered. The influence of the exhaust gas recirculation (EGR) on the intra-cylindric processes, namely on formation of nitric oxides in the hydrogen engine is studied for the first time experimentally and with the help of the mathematical model based on the three-dimensional non-stationary equations of type of Navier-Stokes. The results obtained for the wide ranges of variation of the advance angle of ignition, excess air ratio and rate of EGR confirm that at successful combination of these controllable parameters the problem of minimization of nitric oxides exhausted by the hydrogen engine is removed.

Keywords: hydrogen engine, experiment, 3D modeling, nitric oxides.

1. Introduction
The reciprocating internal combustion engines (RICE) are widespread in the transport and stationary energetics due to, first of all, high efficiency, ensuring minimum (in comparison with other heat engines) specific fuel consumption. It is evident that the prospects for further perfection of RICE are directly related to improvement of their ecological indices. The most reliable way in this direction is the use of alternative fuels, among which hydrogen occupies a special place \cite{1, 2, 3}. Besides the fact that hydrogen reserves are almost inexhaustible, as motor fuel it has remarkable properties that far exceed those of traditional fuels of petroleum origin: the lowest burning heat (approximately 3 times higher), wide range of variation of ignition limits (under atmospheric conditions ignition occurs at an excess air ratio $\alpha_{air}=0.13-10$), high flame propagation rate (for laminar flame under atmospheric conditions in air at $\alpha_{air}=1$, its value is 2.3 m/s, which is about 5-6 times higher compared with traditional fuels), minimum energy for ignition (at $\alpha_{air}=1$ it is equal to 0.017 mJ in air, which is about 14 times less than for traditional fuels) \cite{3}. From the environmental point of view the advantage of hydrogen is that from four harmful substances (nitric oxides NO\textsubscript{x}, soot, carbon monoxide CO and unburned hydrocarbons CH\textsubscript{x}), emission of which is limited by the legislation, the carbon-containing substances and also “greenhouse” gas CO\textsubscript{2} are absent in the exhaust gases of hydrogen RICE. It is clear that improvement of ecological indices of the hydrogen RICE with both, self-ignition \cite{4} and forced ignition \cite{5} implies minimization of the concentration of NO\textsubscript{x} in the combustion products.

In spite of the fact that hydrogen has rapidly spread as a motor fuel in recent years, the combustion process of which leads to significant changes in intra-cylinder processes in comparison with the engines operating on traditional fuels, a number of important problems, in particular, influence of EGR on formation of nitric oxides have not been
practically studied yet. It is obvious that solution of the problem is of practical importance, especially at conversion of serial traditional engines on hydrogen.

The results of the experimental study and 3D mathematical modeling of the working process and formation of nitric oxides in the combustion chamber of hydrogen RICE with external mixing and spark ignition are presented below. With the purpose of minimization of NOx emission, as well as prevention of abnormal combustion processes (detonation, early ignition, back fire) [6, 7], the experimental hydrogen engine operated in the mode $a_{\text{ad}}>1.5$. We note that high heat of hydrogen combustion provides acceptable power indices of the engine at operating on the leaked hydrogen-air mixture. The hydrogen engine under study was also equipped with the EGR system for study its influence on the environmental and effective indices.

2. Brief description of the experimental stand
Experimental researches were carried out on the test bench at the research laboratory of the Beijing Institute of Technology (BIT) [5, 6]. The engine under study is a hydrogen version of the 4-cylinder Chinese made atmospheric gasoline RICE CA20 with electronic, multipoint converted on hydrogen in BIT, technical data of which are given in Table 1. We note that the experimental hydrogen engine retains the basic parameters of the base engine CA20 without significant changes. In contrast to base gasoline RICE, where independent ignitions have the pairs of cylinders (1-4 and 2-3), in order to prevent misfires that can occur at operating on hydrogen-air super-leaked mixture, an independent ignition is used on the hydrogen engine for each cylinder. Besides, the system of hydrogen gas supply into the inlet system is changed. Considering the low hydrogen density and its high volumetric flow rate required for providing the necessary power of the engine, two hydrogen injectors are installed on each cylinder, i.e. an injector is located in each inlet. The hydrogen cyclic supply and excess air ratio are monitored, controlled and registered for each mode of operation during the experiment. The basic technical data of the experimental hydrogen RICE: Number of cylinders – 4; Diameter of the cylinder D=86 mm; Degree of compression $\varepsilon=10$; Cooling system – Water; Rated power $N_\text{r}=60$ kW at frequency of rotation $n=5000$ min$^{-1}$; Maximum torque $M_\text{r}=111$ Nm at frequency of rotation n=4000 min$^{-1}$.

The experimental bench is equipped with a measuring system ensuring measurement of all the necessary parameters (power, torque, fuel consumption, frequency of rotation of the crankshaft) [5, 6]. The devices for special measurements are also installed on the bench, primarily for indicating the engine and determining emission of the nitric oxides. The measured frequencies of rotation of the engine and pressure in the cylinder are introduced into the combustion analyzer for determining the heat release rate.

3. 3D model of intra-cylinder processes of the hydrogen RICE
The mathematical model of non-stationary turbulent transfer processes is based on the fundamental equations of momentum (Navier-Stokes), energy (Fourier-Kirchhoff), concentration (Fick) and continuity [4, 8, 9], averaged according to the method of Favre and using density $\rho$ as a weight function [9, 10]. These equations of transfer, as a result of averaging, take the form of Reynolds:

\[
\begin{align*}
\rho \frac{Dp}{Dt} &= \sum_{i=1}^{3} \rho \frac{\partial \bar{W}_i}{\partial x_i} + \rho G_i - \frac{\partial}{\partial x_i} \left( \mu \frac{\partial \bar{W}_i}{\partial x_i} + \frac{\partial \bar{W}_j}{\partial x_i} \right) - \frac{2}{3} \rho S_{ij} \frac{\partial \bar{W}_k}{\partial x_k} - \rho W_i ' W_j ' ; \\
\rho \frac{D\bar{W}_i}{Dt} &= \sum_{j=1}^{3} \rho \frac{\partial \bar{W}_j}{\partial x_j} + \frac{\partial \bar{W}_i}{\partial x_j} \left( \tau_{ij} \bar{W}_j \right) + \frac{\partial}{\partial x_j} \left( \lambda \frac{\partial \bar{W}_i}{\partial x_j} - c_p \rho \bar{T} ' W_j ' \right) + \bar{W}_j ' Q_i ' + \frac{\partial \bar{q}_{\text{th}}}{\partial x_j} ; \\
\frac{\partial \tilde{\rho}}{\partial t} &+ \frac{\partial \bar{W}_i}{\partial x_i} \left( D_{ij} \frac{\partial \tilde{\rho}}{\partial x_j} - \bar{C}_{ij} W_j \right) + \bar{m} = 0 ,
\end{align*}
\]  

where $D/Dt$ is a substance derivative; $\rho$ – density of the working body (WB), kg/m$^3$; $p$ – pressure of WB, Pa; $G_i$ – projection of density vector of volumetric forces, N/m$^3$ on the axes $Ox_i$ of the rectangular Cartesian coordinate system;
C – concentration, kg/m$^3$; H – total specific energy, J/kg; $\mu$ – dynamic viscosity, kg/(m$\cdot$S); $c_p$ – thermal capacity at constant pressure, J/(kg·K); $w_r$ – rate of the chemical reaction per unit volume, kg/(m$^3$·S); $Q_r$ – amount of released heat per unit mass, J/kg; $\lambda$ – thermal conductivity, W/(m·K); $\delta_{ij}$ – Kronecker symbol; $D$ – diffusion coefficient, m$^2$/S; $\dot{m}$ - intensity of the mass source (rate of change of the chemical component mass in unit volume), kg/(m$^3$·S); $W$ – velocity vector. The dashed parameters denote turbulent pulsations and the averaged parameters are denoted with a dash on top.

The system of the equations of Reynolds is ended by the $k$-$\zeta$-$f$ model of turbulence specially developed for modeling of processes in the piston engines [11]. For describing the processes in the near-wall layers are used so-called near-wall functions [9, 11].

The combustion process is taken into account by intensity of the internal heat source $q_v$, W/m$^3$ and mass expenditure $\dot{m}$, kg/(m$^3$·S). The values of these parameters can be calculated using rate $w_r$ of the chemical combustion reaction [3.9]: $q_v = Q_r w_r$; $\dot{m} = -w_r$, where $Q_r$ is amount of the heat per unit mass released as a result of the chemical reaction, J/kg. The rate of the combustion process is determined on the base of the coherent flame model (CFM) described in [9]. The formation of nitric oxides [NO$_x$] is modeled on the base of the extended mechanism of Y. B. Zeldovich [9]. We note that the concentration is donated here and further by square brackets. The described 3D-mathematical model of intra-cylinder processes is realized with the help of the CRFD program FIRE, developed by AVL List GmbH (Austria) [9]. The FIRE kernel is based on the numerical method of control volumes using the advanced algorithm SIMPLE. Sampling of the transfer equation (1) is carried out using interpolation circuit of the second order of accuracy, which is optimal, both in accuracy and in time of counting.

4. The results of calculation and experimental studies

Verification of the mathematical model of intra-cylinder processes of hydrogen RICE, based on equations (1), was carried out by comparing the results of modelling with experimental data. In particular, were compared the experimental and calculated indicator diagrams, as well as changes in temperature of the working body and heat release rates obtained on their basis. Despite the good congruence of these parameters (the difference between the experimental and calculated values of instantaneous parameters did not exceed: by pressure and temperature 1 - 3%, by heat release rate 10 - 12%), for evaluation of reliability of the developed 3D mathematical model, comparisons were made of the concentrations of the final product of the working process - nitric oxides obtained by direct measurement in the outlet system of the hydrogen RICE and modelling.

![Figure 1. Influence of the advance angle of ignition on the emission of nitric oxides (1. Modeling, %, 2. experiment). The mode of operation of the hydrogen RICE, n=3000 min$^{-1}$.](image1)

![Figure 2. Change of heat release rate $dQ_r/d\phi$ in the hydrogen RICE depending on the advance angle of ignition at operation mode of the hydrogen RICE n = 3000 min$^{-1}$ (1. $\varphi_u=25^\circ$; 2. $\varphi_u=20^\circ$; 3. $\varphi_u=15^\circ$; 4. $\varphi_u=10^\circ$; 5. $\varphi_u=5^\circ$), obtained as a result of processing of the experimental indicator diagrams.](image2)

We note that the verification of the 3D model was carried out in the wide range of changes in frequency of rotation of the engine, EGR degree, excess air ratio and advance angle of ignition. When converting the traditional RICE (in
this case, gasoline) to hydrogen, it becomes necessary to ascertain the optimal (from the point of view of the ecological compatibility and fuel economy of the engine) advance angle of ignition $\varphi_a$. The results of the modeling and experimental study of influence of $\varphi_a$ on emission of NO are given in Figure 1. The maximum deviation of the results of modeling from the experimental data, as shown, does not exceed 11%. Analysis of the experimental indicator diagrams and obtained on their basis heat release rates $dQ_x/d\varphi=f(\varphi)$ (Figure 2) indicates that for this mode of operation of the engine the most optimal is the advance angle of ignition $\varphi_a=15^\circ$.

The positions of these peak values relative to the upper dead point at $\varphi_a=15^\circ$ are the most favorable that indicates the efficiency of the working cycle of the hydrogen engine (indicator efficiency at this mode according to the experimental data $\eta_i=40.8\%$). It is obvious that this is the result of intensification of the combustion process, leading simultaneously to the rise in $p_z$ and increase in both, the maximum cycle temperature (in this case $T_z=2375$ K) and local temperatures at the flame front. The increase in the temperature level of the cycle is, of course, accompanied by the increase of emission of nitric oxides. This explains the increase of [NOx] with increase of $\varphi_a$ (Figure 1).

For the first time on the hydrogen RICE was studied the influence of the EGR on the working process of the hydrogen RICE. The experimental results given in Figure 3 show that the use of EGR (degree of recycling $z=15\%$) at $n = 1000$ min$^{-1}$ results in the significant reduction in emission of NOx (almost 3 times). It can also be seen that with increase of $\alpha_v$ the maximum emission compared to the combustion process without EGR, moves away relatively further from the stoichiometric value $\alpha_v=1$. Besides, the changes of [NOx] depending on $\alpha_v$ occur more smoothly, than for the case without EGR (Figure 3). Figure 4 shows the changes in concentrations of nitric oxides in the exhaust gases of the hydrogen engine under study, depending on the excess air ratio at frequency of rotation of the crankshaft $n = 3000$ min$^{-1}$ and degree of EGR $z=15\%$, obtained experimentally and by modeling, that confirm the reliability and trustworthiness of the developed 3D model of the intra-cylinder processes. It is noticeable that the maximum amount of nitric oxides during hydrogen combustion is formed at slightly enriched hydrogen-air mixture ($\alpha_{air}=1,1…1,2$) and its value relatively little depends on the frequency of rotation of the crankshaft. However, as already noted, the operation of the hydrogen engine at $\alpha_{air}=1,1…1,2$ or close to these values, is not desirable due to the danger of detonation combustion, back fires and early ignition [6,7].

![Figure 3](image1.png)
**Figure 3.** The results of the experimental study of the nitric oxides emission depending on degree of EGR ($1. z=0, 2. z=15\%$). Operation mode of the hydrogen RICE, $n = 1000$ min$^{-1}$.

![Figure 4](image2.png)
**Figure 4.** Influence of the excess air ratio on the emission of nitric oxides at constant frequency of rotation of the crankshaft $n = 3000$ min$^{-1}$ and degree of EGR, $z=15\%$ ($1. \text{modeling, 2. Experiment.}$)

The results of the study showed that the effect of the excess air ratio is more significant than that of the frequency of rotation. At low frequency of rotation of the engine $n = 1000$ min$^{-1}$ (when $\alpha_{air}$ decreases from 2.0 to 1.2), the concentration of nitric oxides in the exhaust gases increases from 200 ppm to its maximum value (approximately 6000 ppm) respectively. In general, judging by the nature of the change in the dependence $[\text{NO}_x]=f(\alpha_{air})$, the formation of nitric oxides in the hydrogen engine occurs similarly to the engines operating on traditional oil fuels in the whole speed range [8]. Absence of the free oxygen at combustion of enriched mixture ($\alpha_{air}<1,0$) and temperature decrease at combustion of leaked mixture ($\alpha_{air}>1,0$) prevent combination of the nitrogen and oxygen and limit formation of
nitric oxides. Obviously, increasing the deviation of $\alpha_{air}$ in any direction from the stoichiometric value ($\alpha_{air}=1.0$) exacerbates this effect. The two characteristic areas of sharp reduction of NO$_x$ depending on $\alpha_{air}$ are clearly seen in Fig. 4:

1. Area of the air excess ratio reduction from $\alpha_{air}=1.1...1.2$ to $\alpha_{air}=0.9$;
2. Area of the air excess ratio rise from $\alpha_{air}=1.1...1.2$ to $\alpha_{air}=2.0$.

At the same time, the second area is about 2 times higher than the first one in the range of change of $\alpha_{air}$ and the change of [NO$_x$] occurs more slowly in it than in the first area. The reduction of [NO$_x$] by increasing $\alpha_{air}$ (super-leaked hydrogen-air mixtures) or by decreasing $\alpha_{air}$ (super-enriched hydrogen-air mixtures) beyond the mentioned limits of change of $\alpha_{air}$ occurs much slower. The presence of areas of sharp reduction (or sharp increase) of [NO$_x$] is explained by the presence of a high temperature – the result of the hydrogen combustion having a high combustion heat and by the peculiarity of changing this temperature in these areas. In this case, in the first zone (in the zone of rich mixtures) there is a high concentration of hydrogen H$_2$ in the cylinder, which is chemically more active than nitrogen N$_2$. Therefore, it reacts faster than N$_2$ with oxygen O$_2$, the amount of which in the rich mixture is small that leads to the sharp decrease in emissions of NO$_x$ (Figure 4). In the second zone, with increase of $\alpha_{air}$ towards super-leaked mixtures, with increase of the air amount, the temperature of the working body decreases in the cylinder, however, the rate of the temperature decrease is lower here than in the first one, and the rate of change of NO$_x$ (Fig.4) correlates with the rate of the temperature change.

Both, the experimental studies and simulations showed that even with a substantially leaked mixture ($\alpha_{air}=1.5$) and degree of EGR, $z=15\%$, the emission of nitric oxides in the exhaust gases of the hydrogen RICE under study is quite high ([NO$_x$]=2000 ppm) (Fig. 4). The further increase in the degree of EGR, $z \geq 20\%$ can lead to the noticeable decrease in effective indices of the engine. It should be noted that the capabilities of the EGR in hydrogen engines have not been practically studied to date. Obviously, the exhaust gas in this case is water vapor H$_2$O, which, when entering the inlet system and stirring with the cooler hydrogen-air mixture, can partially condense, and then evaporate again with increase of the temperature during the compression process. This can lead to the drop of temperature in the cylinder and decrease of nitric oxides similarly to the engines with water injection into the cylinder [12]. Obviously, the temperature of the exhaust gases bypassed into the hydrogen engine inlet system can play a role here. Indeed, according to the results of measurement at the mode $n=1000$ min$^{-1}$, we have $t_{up}=431^\circ$C, which is approximately 1.6 times less than the temperature $t_{up}=679^\circ$C at $n=4500$ min$^{-1}$ with the almost unchanged composition ($\alpha_{air}=1.61 – 1.64$) of the hydrogen-air mixture. The exhaust gases presenting water vapour, with such temperatures enter the inlet system having atmospheric parameters $p_0$ and $t_0$, where the steam condensation temperature is equal to $t_{atm}=100^\circ$C. Under such conditions, due to the lack of time, the steam can presumably only partially condense before entering the cylinder. During the compression stroke, the steam condensation process continues until the temperature in the cylinder reaches the boiling point (condensation) of water (about 180$^\circ$C at 10 bars). The water vapor not a reactive gas and is not involved in the combustion process, but its presence in the cylinder, both as gas and condensed water, leads to decrease in the temperature of the working body and consequently, to decrease in the emission of nitric oxides. Thus, the EGR process in the hydrogen engine is accompanied by the phenomena similar to the process in the engines in combustion chambers of which water is injected for reduction of NO$_x$ emissions.

5. Conclusion
The results of the experimental study, as well as the mathematical modeling of the working process of the hydrogen engine with injection of hydrogen gas into the inlet system and ignition of the hydrogen-air mixture using an electric spark, allow us to conclude that the choice of the excess air ratio $\alpha_{air}$ is the most important factor for preventing abnormal phenomena (back fire, early ignition, detonation combustion) and reduction of the nitric oxides content in exhaust gases, as well as ensuring normal, stable engine operation. It is confirmed that there is a relationship between $\alpha_{air}$ and emission of nitric oxides NO$_x$, which is relatively little dependent on the engine speed mode. It is established
that in the limits of change of air excess ratio $\alpha_{\text{air}}=1.6-2.4$, within the range of change of frequency of rotation of the crankshaft speed ($n = 1000-5000 \text{ min}^{-1}$) the stable operation of hydrogen engine is provided without abnormal phenomena and misfires. The speed characteristic of the hydrogen engine, built with a fully open air throttle, when at all modes the condition of constancy of the excess air ratio ($\alpha_{\text{air}} \approx 1.6-1.7$) was observed, showed that the minimum specific effective hydrogen flow rate $g_{\text{emin}}=87.24 \text{ g/(kWh)}$ was reached at $n = 2500 \text{ min}^{-1}$. In idling mode, the specific flow rate of hydrogen reaches 96 g/(kWh). In mode $n = 5000 \text{ min}^{-1}$, we have $g_e=92.2 \text{ g/(kWh)}$ and $N_e=51.0 \text{ kW}$. Achieving such a maximum power on the experimental hydrogen engine is possible at $\alpha_{\text{в}}=1.35$ in mode $n = 5500 \text{ min}^{-1}$, but in this case the signs of abnormal combustion appear. They are expressed primarily in appearance of back fires due to the high temperature of the residual combustion products and in high speeds of movement of the flame front. The latters lead to increase in the rates of heat release and pressure, observed during the analysis of indicator diagrams. A study of influence of EGR on the working process, conducted for the first time for hydrogen RICE, shows that its use during the engine operation on the leaked hydrogen-air mixture ($\alpha_{\text{air}}>1.6$) practically eliminates the problem of NO$_x$ emission. A verification of the 3D model of the working process of the hydrogen engine was carried out based on the results of experimental studies of the hydrogen engine and fundamental equations of three-dimensional non-stationary turbulent transfer, in a wide range of changes in the controlled and mode parameters of the engine. This model, successfully tested earlier for a hydrogen diesel [3, 4, 10], was first used for the hydrogen engine with spark ignition. Good coincidence of the results of modeling and experimental data, especially on indicator diagrams and emissions of nitric oxides, obtained by changes in such engine parameters as advance angle of ignition; excess air ratio and degree of EGR, makes it possible to conclude that in the form of a verified model a tool has been created for conducting numerical experiments on study of intra-cylinder processes, environmental and efficient characteristics of promising hydrogen engines with forced ignition. The use of this model can significantly reduce the time and cost of creation of promising ICE of this type.

On the whole, the effectiveness of operation of the engine with spark ignition on the leaked hydrogen-air mixtures and expediency of its creation have been confirmed. An instrument in the form of a verified 3D mathematical model has been developed for further research and improvement of the working process of this engine.

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