Improvement of ecological characteristics of the hydrogen diesel engine

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Abstract. In the article are considered the questions of influence of a swirl intensity of the shot and injector design on the ecological indices of the hydrogen diesel, little-investigated till now. The necessity of solution of these problems arises at conversion of the serial diesel engine into the hydrogen diesel. The mathematical model consists of the three-dimensional non-stationary equations of transfer and also models of turbulence and combustion. The numerical experiments have been carried out with the use of program code FIRE. The optimal values of parameters of the working process, ensuring improvement of the effective and ecological indices of the hydrogen diesel are determined.

1. Introduction

The problems of preservation of the environment and providing the transport with power are the basic problems for the modern civilization. These problems are directly connected with piston engines - the basic users of natural fuels, playing an essential role in the atmospheric pollution.

It is necessary to underline that soot is practically absent in combustion residues of the hydrogen diesel engine that against toughening acts on ecology is the main advantage in comparison with the diesel engine conversion into the gas-diesel [1]. In this connection, improvement of the ecological indices of the hydrogen diesel, first of all, means decrease of nitrogen oxides concentration.

The aim of this work is to study such little-investigated questions solution of which is necessary at conversion of the serial diesel engine into the hydrogen diesel: Influence of the injector construction on the ecological indices of the hydrogen diesel engine and determination of the air swirl motion optimal intensity.

2. Mathematical model of the hydrogen diesel engine working process

The model of the operating process proceeding in the cylinder of a hydrogen diesel engine is constructed taking into account the turbulent ignition processes and the chemical kinetics of formation of the nitrogen oxides [2, 3, 4]. The model is based on the generalized transfer equation, the vector and tensor forms of which are given in the table 1. In this equation Φ is one of the dependent variables, Γ_Φ - generalized transfer coefficient (of diffusion, viscosity, thermal, and temperature conductivity), S_Φ - the source term. At substitution of the relevant expressions from the table into the generalized equation a system of three-dimensional nonstationary transfer equations is obtained: equations of momentum (Navier-Stokes), equations of energy (Fourier-Kirchhoff), and equations of continuity and diffusion (Fick). The following notation is assumed in the equations from the table 1: $D/D\tau$ - substantial derivative;

$\mathbf{W}$ - vector of the gas velocity (m/s); ρ - density of the gas (kg/m^3); p - pressure (N/m^2); G_i - projection of the vector of density of volume forces (N/m^3) on axis Ox_i of the Cartesian coordinate system; C - concentration (kg/m^3); H - total specific energy (J/kg); $V_\mu = \frac{1}{3}\mu \cdot grad\left(div\,\vec{W}\right)$ - term representing volume deformation; μ - dynamic viscosity (kg/(m s)); c_p - thermal capacity at constant pressure (J/(kg K)), w_r - velocity of the chemical reaction per unit volume (kg/(s m^3)); Qr - amount of heat educed per unit of mass (J/kg); λ - heat conductivity (W/(m K)); δ_{ij} - Kronecker symbol; D_c - diffusion coefficient (m^2/s); $\dot{m}$ - intensity of the mass source, the rate of the change of mass of the chemical component per unit volume (kg/(s m^3)). The radiation heat flux $\dfrac{\partial q_{Rj}}{\partial x_j}$ from the radiation source plays a substantial role only in the heterogeneous combustion of the liquid diesel fuel, which is accompanied by the intensive formation of the solid microparticles of soot - main generators of radiation. In case of the hydrogen burning the water steam is the basic source of thermal radiation whose selective radiation is negligibly small [5, 6, 7, 8].

As a result of averaging according to the Favre method [9] the original system of equations of three-dimensional nonstationary transfer is transformed into the system of Reynolds equations containing new unknown quantities with turbulent fluctuations of the parameters (see table 1). A relatively new k–ζ–f model of turbulence is used to close the Reynolds system [10].

Table 1. The basic equations of mathematical model of the working process of a hydrogen diesel engine.

<table>
<tr><td colspan="3" align="center">EQUATIONS OF LAWS OF CONSERVATION AS PARTICULAR CASES
OF THE GENERALIZED DIFFERENTIAL EQUATION</td></tr>
<tr><td colspan="3" align="center">$\dfrac{\partial}{\partial \tau}\left(\rho\Phi\right) + div\left(\rho\,\vec{W}\Phi\right) = div\left(\Gamma_\Phi\,grad\Phi\right) + S_\Phi \quad \Leftrightarrow \quad \dfrac{\partial}{\partial \tau}\left(\rho\Phi\right) + \dfrac{\partial}{\partial x_j}\left(\rho W_j\Phi\right) = \dfrac{\partial}{\partial x_j}\left(\Gamma_\Phi\,\dfrac{\partial\Phi}{\partial x_j}\right) + S_\Phi$</td></tr>
<tr>
<td rowspan="4">$\Phi = W_i,\ \Gamma_\Phi = \mu,$

$S_\Phi = G_i - \dfrac{\partial p}{\partial x_i} + V_\mu$

.

Equation of conservation of the momentum (Navier–Stokes equation)</td>
<td>Initial form</td>
<td align="center">$\rho\dfrac{DW_i}{D\tau} = G_i - \dfrac{\partial p}{\partial x_i} + \dfrac{\partial}{\partial x_j}\left[\mu\left(\dfrac{\partial W_i}{\partial x_j} + \dfrac{\partial W_j}{\partial x_i} - \dfrac{2}{3}\delta_{ij}\dfrac{\partial W_k}{\partial x_k}\right)\right]$</td>
</tr>
<tr>
<td>Reynolds form</td>
<td align="center">$\bar{\rho}\dfrac{D\overline{W}_i}{D\tau} = \overline{G}_i - \dfrac{\partial\overline{p}}{\partial x_i} + \dfrac{\partial}{\partial x_j}\left[\mu\left(\dfrac{\partial\overline{W}_i}{\partial x_j} + \dfrac{\partial\overline{W}_j}{\partial x_i} - \dfrac{2}{3}\delta_{ij}\dfrac{\partial\overline{W}_k}{\partial x_k}\right)\right] - \overline{\rho\,\overline{W_i'W_j'}}$</td>
</tr>
<tr>
<td rowspan="2">New unknown quantities</td>
<td align="center">$\overline{\rho\,\overline{W_i'W_j'}}$ - tensor of the Reynolds turbulent stresses determined by the oscillatory components of velocity;</td>
</tr>
<tr>
<td align="center">$\overline{\tau_{ij}} = \mu\left(\dfrac{\partial\overline{W}_i}{\partial x_j} + \dfrac{\partial\overline{W}_j}{\partial x_i} - \dfrac{2}{3}\delta_{ij}\dfrac{\partial\overline{W}_k}{\partial x_k}\right)$ - tensor of the viscous (turbulent) stresses determined by the averaged values of the velocity components.</td>
</tr>
</table>

Table 1. (Continued)

$\Phi = H$, $\Gamma_\Phi = \dfrac{\lambda}{c_p}$, $S_\Phi = \dfrac{\partial p}{\partial \tau} + \dfrac{\partial}{\partial x_i}\left(\tau_{ij} W_j\right) + + G_j W_j + w_r Q_r + \dfrac{\partial q_{R_j}}{\partial x_j}$ Energy conservation equation	Initial form	$\rho \dfrac{DH}{D\tau} = G_j W_j + \dfrac{\partial p}{\partial \tau} + \dfrac{\partial}{\partial x_i}\left(\tau_{ij} W_j\right) + \dfrac{\partial}{\partial x_j}\left(\lambda \dfrac{\partial T}{\partial x_j}\right) + w_r Q_r + \dfrac{\partial q_{R_j}}{\partial x_j}$
	Reynolds form	$\bar{\rho}\dfrac{D\overline{H}}{D\tau} = \overline{G_j W_j} + \dfrac{\partial \bar{p}}{\partial \tau} + \dfrac{\partial}{\partial x_j}(\overline{\tau_{ij}}\,\overline{W_j}) + \dfrac{\partial}{\partial x_j}\left(\lambda \dfrac{\partial \overline{T}}{\partial x_j} - c_p \bar{\rho}\overline{T'W_j'}\right)$ $+ \overline{w_r Q_r} + \dfrac{\partial \overline{q}_{R_j}}{\partial x_j}$
	New unknown quantities	$c_p\;\overline{\rho}\;\overline{T'W_j'}$ - is turbulent enthalpy transfer $\overline{\rho}\,c_p T'$ by means of velocity fluctuation W_j';
$\Phi = 1$, $\Gamma_\Phi = 0$, $S_\Phi = 0$ Mass (continuity) conservation equation	Initial form	$\dfrac{\partial p}{\partial \tau} + \dfrac{\partial}{\partial x_i}\left(\rho W_j\right) = 0$
	Reynolds for	$\dfrac{\partial \bar{p}}{\partial \tau} + \dfrac{\partial}{\partial x_i}\left(\bar{\rho}\overline{W}_j\right) = 0$
$\Phi = \dfrac{C_l}{\rho}$, $\Gamma_\Phi = D_l \rho$, $S_\Phi = \overset{\bullet}{m_l}$. Diffusion (concentration) equation	Initial form	$\dfrac{DC}{D\tau} = \dfrac{\partial}{\partial x_j}\left(D\dfrac{\partial C}{\partial x_j}\right) + \overset{\bullet}{m}$
	Reynolds form	$\dfrac{D\overline{C}}{D\tau} = \dfrac{\partial}{\partial x_j}\left(D\dfrac{\partial \overline{C}}{\partial x_j} - \overline{C'W_j'}\right) + \overline{\overset{\bullet}{m}}$,
	New unknown quantities	$\overline{C'W_j'}$ - turbulent diffusion transfer of concentration C_l of component ℓ by means of the velocity fluctuation W_j'.

In the equations is used, the rule of summation according to the twice-repeating index $i, j, k = 1,2,3$ and averaging is realized according to Favre; i.e ,the density is used as a weight function.

The wall functions are used to describe the flow of the working medium and heat exchange in the wall zone [11]. The process of turbulent combustion is simulated on the base of the well-known model of Magnussen–Hjertager [4, 12], which has also been well tested in the theory of piston engines. Its advantage is that there are no turbulent fluctuations of parameters in it. The model assumes that combustion of the fuel and air mixture occurs instantly and consequently the average combustion rate is determined by the time of turbulent mixing of the reagents and is written as follows:

$$\bar{w}_r = \frac{A}{\tau_t}\bar{\rho}\,min\left(\overline{m}_T, \frac{\overline{m}_{o_2}}{L_0}, \qquad B\frac{\overline{m}_{comb.pr.}}{1+L_0}\right), \tag{1}$$

where L_0 is the bulk stoichiometric quantity of air; $\tau_t = \bar{k}/\bar{\varepsilon}$ - time scale of turbulent mixing; A and B - empirical coefficients that take into account the influence of turbulence and fuel parameters on the rate of the chemical reaction. It is evident that for the concrete conditions they should be specified according

to the experimental data. We note that the experimental indicator diagrams of the hydrogen diesel engine under study were used for their determination.

The local formations of the nitrogen oxides in the combustion chamber of the hydrogen diesel engine are simulated with the use of the extended mechanism of Zeldovich [4, 13], developed for NO whose portion in the total concentration of all nitrogen oxides [NOx] in the piston engines is 90% and more [4]. In this connection it is assumed that [NO$_x$] ≡ [NO].

The model was numerically realized on the base of the 3D-CFD code FIRE developed by the AVL List GmbH [14], designed for numerical solution of specific problems of the theory of piston engines. The core of the FIRE is based on the numerical method of control volumes with the use of the improved algorithm SIMPLE described in detail in [2, 14].

3. Model verification

The research objects were the experimental, four-stroke, single-cylinder supercharged diesel engine with direct injection of the gaseous hydrogen and its basic variant with injection of the diesel fuel. The experimental diesel engines were single-cylinder sections of the series diesel engines MAN with a ratio of piston stroke/cylinder diameter $S/D = 30/24$ cm/cm and a crankshaft rotation rate of $n = 800$ min^{-1}. The injection pressures were $pi_{nj} = 350$ bar and $p_{inj} = 300$ bar, and the degrees of compression were ε= 13,5 and ε=17 for the basic and hydrogen diesel engines, respectively [15, 16].
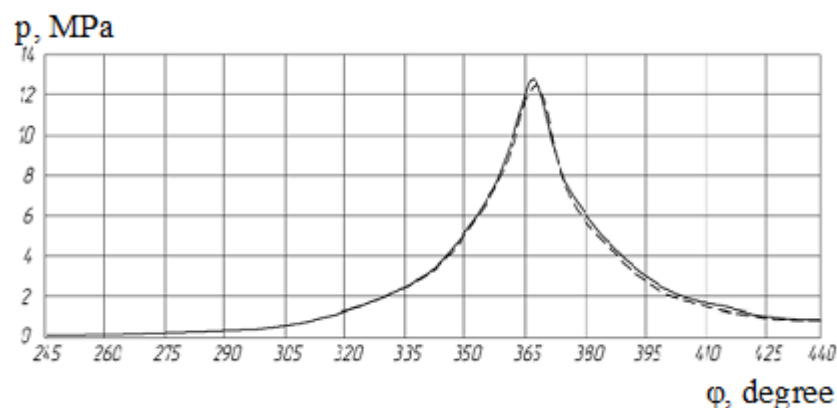
Figure 1. Indicator diagrams of the hydrogen diesel engine: experiment (- - -) and 3D modelling (−). Factors in the model of combustion (1) A=10, B=1. φ – angle of rotation of the crankshaft (ARC).

The model of operating process of the hydrogen diesel engine is verified by comparing the results of the numerical calculation with the experimental data (figure 1). The values of the empirical coefficients $A = 10$ and $B = 1$ were determined in the Magnussen-Hjertager combustion model (1), which closely correlate the experimental indicator diagrams with the calculated data (the difference in the maximum pressure of the cycle did not exceed 2 %). It should be noted that a comparative analysis of the operating processes of the basic and hydrogen diesel engines was carried out at approximate equality of the effective horse powers.

Some studies on the selection of certain structural (structure of the injection nozzle, swirl intensity of the charge) parameters having influence on the local formation of the nitrogen oxide in the combustion chamber were carried out to improve the ecological indices of the hydrogen diesel engine.

4. Influence of the injector design on formation of the nitrogen oxides

A series of numerical experiments carried out for variants of the injection nozzle has shown that the maximum and minimum values of the total mass portions of nitrogen oxides per cycle in terms of the cylinder volume are obtained with the use of nozzles 6×0,7 mm and 18×0,5 mm (z × d$_c$ _ number of nozzle holes z and the nozzle hole diameter d$_c$ in mm) and amount to [NO$_x$]$_\Sigma$= 0,00158 and

$[NO_x]_\Sigma$=0,00027 respectively. The remaining nozzles give the intermediate results (figure 2). It is seen that with increase of the number of injection nozzle holes, hydrogen is more uniformly distributed over the volume of the combustion chamber, the hydrogen-air mixture is homogenized and the level of local temperatures in the combustion areas decreases that leads to decrease in concentration of NOx.
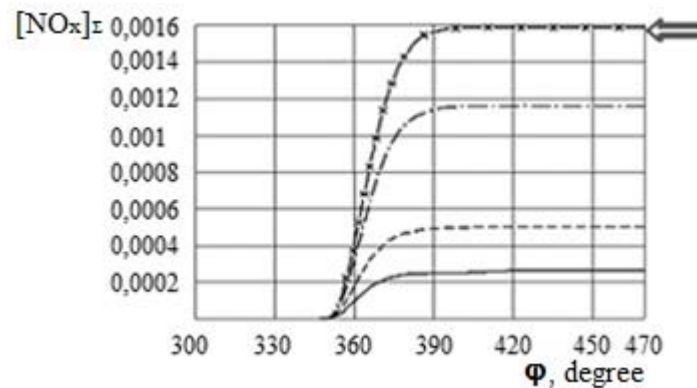
Figure 2. The total concentrations of the nitrogen oxides for different structures of the spray unit: 1. (— x —) 6×0,7 mm; 2. (— • —) 4×0,5 mm + 4×0,7 mm; 3. (- - - -) 12×0,5 mm; 4. (—) 18×0,5 mm. The arrow shows the experimental value for the nozzle 6×0,7 mm. φ – angle of rotation of the crankshaft (ARC).

5. Influence of intensity of the air whirl on formation of the nitrogen oxides
Usually, the whirling motion of the charge, together with the characteristic of fuel injection and the nozzle structure, ensures a high-quality proceeding of the carburetion and ignition processes, and first of all decrease of the ignition delay. It is possible to achieve the low specific fuel consumption at the optimal intensity $D_n=n_{air}/n$ (n_{air} - frequency of the air whirling motion, n - frequency of the crankshaft rotation) of the whirling motion. On the other hand, it leads to increase of the NO_x emission. The influence of the whirling motion on formation of the nitrogen oxides in the hydrogen diesel engine has a completely different character (figure 3). The numerical experiments showed that a significant increase in the air whirl at the end of compression contributes to fast diffusion with the hydrogen. Already at the onset of supply, the hydrogen is diluted by air, so that its amount in the local areas turns out to be lower than the concentration ignition limits (less than 4% by volume). Self-ignition starts later after the hydrogen concentration increases. It should be noted that at the same time the ignition delay increases [17, 18, 19], the combustion process is delayed, the maximum velocity of heat generation moves away from the upper dead point (UDP), the local temperatures of the working medium decrease, and, as a result, the nitrogen oxide emission decreases (figure 3). In addition, the delayed energy conversion process leads to decreased rate of increase of the pressure and reduction of noise. However, such a change in the heat generation velocity leads to decrease in the efficiency of the cycle. Thus, increase of the charge whirling motion intensity in the hydrogen diesel engine leads to worsening of its efficiency indices.
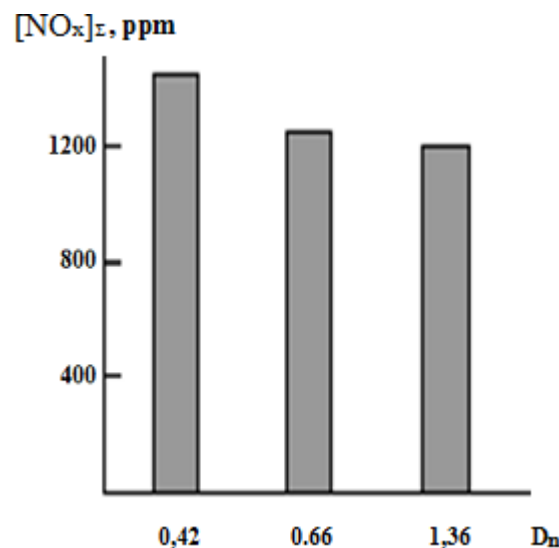
Figure 3. Influence of intensity of the charge whirling motion on the concentration of the nitrogen oxides in the products of combustion of the hydrogen diesel. The average effective pressure p_e=8,5 bar; frequency of rotation of the crankshaft n=800 min^{-1}; the air excess factor $\lambda_{air.}$=2,4_2,5; angle of outstripping of the hydrogen injection $\varphi_{inj.}$=15^0; the air temperature and pressure at the inlet T_k=296 K и p_k=1,29 bar; nozzle №1 (6×0,7 mm).

5. Conclusions

Out of the possible methods of converting the serial diesel engines into the hydrogen ones, the concept of the hydrogen diesel engine operating by self-ignition of the gaseous hydrogen is promising. The main problem of improving the ecological indices of the hydrogen diesel engine is minimization of the nitrogen oxide emission, which can be realized by changing the structural and regulating parameters.

The optimal (from the standpoint of efficiency and environmental compatibility) combination of the operating process parameters for the stationary hydrogen diesel engine under study is: spray 18×0,5 mm for the hydrogen supply; cyclic supply of the hydrogen m_c=0,49 g/cycle; the air excess factor λ_{air}=2,5. In this case, the concentration of the nitrogen oxides in the products of combustion is $[NO_x]_\Sigma$=950 ppm, and the indicator efficiency of the hydrogen diesel engine η_i=0,48 that is quite admissible for this type of the diesel engine.

Acknowledgement

References

[1]   Kavtaradze R Z 2011 *Thermal-Physical Processes in Diesel Motors Converted to Natural Gas and Hydrogen* (In Russian) (Moscow: Bauman State Technical University Publishing House) p 238
[2]   Andersen D Tannehil G and Pletcher R 1984 *Computational fluid mechanics and heat transfer* (Hemisphere Publishing Corporation: New York, Cambridge, Sydney) p 776
[3]   Merker G, Schwarz Ch, Stiesch G et al, 2016 *Verbrennungsmotoren. Simulation der Verbrennubg und Schadstoffbildung* 3 Auflage (Teubner-Verlag: Stuuugart, Leipzig, Wiesbaden) p 820
[4]   Kavtaradze R Z 2016 *Theory of Piston Engines. Special chapters*. Second edition (In Russian) (Moscow: Bauman State Technical University Publishing House) p 590

[5]   Kavtaradze R Z 2016 *Local heat exchange in piston engines*. Third edition (In Russian) (Moscow: Bauman State Technical University Publishing House) p 515

[6]   Kavtaradze R Z, Gaivoronskii A I and Fedorov V A et al 2007 Calculation of Radiative-Convective Heat Transfer in the Combustor of Diesel Engine. *High Temperature* vol 45 No 5 pp 673-80

[7]   Kavtaradze R Z, Onishchenk D O and Zelentsov A A et al 2009 The influence of rotational charge motion intensity on nitric oxide formation in gas-engine cylinder *International Journal of Heat and Mass Transfer* 52 pp 4308–16

[8]   Kavtaradze R, Zelentsov A, Gladyshev S et al 2012 Heat Insulating Effect of Soot Deposit on Local Transient Heat Transfer in Diesel Engine Combustion Chamber *SAE International Paper* p 12

[9]   Favre A 1965 Equations des Gaz Turbulents Compressibles *1. Formes Generales. J. Mecanique.* vol 4 pp 361-90

[10]   Hanjalič K, Popovač M Hadziabdič M et al 2004 Near -Wall Elliptic-Relaxation Eddy-Viscosity Turbulence Model for CFD *Int. J. Heat Fluid Flow* No 25 p 897

[11]   Popovač M and Hanjalič K 2005 Compound Wall Treatment for RANS Computation of Complex Turbulent Flow. *Proc. 3rd Int. Conf. on Comput. Fluid and Solid Mechanics* pp 1-28

[12]   Magnussen B F and Hjertager B H 1976   On Mathematical Models of Turbulent Combustion with Special Emphasis of Soot Formation and Combustion *16th Int. Symp. on Combustion. Cambridge.* pp 719-29

[13]   Warnatz J, Maas U and Dibble R 2001 *Verbrennung: Physikalisch-Chemische Grundlagen, Modellierung und Simulation, Experimente, Schadstoffentstehung* 3. Auflage (Berlin: Heidelberg: Springer-Verlag) p 326

[14]   2016 FIRE *Users Manual Version 2016* (Graz, Austria: AVL List GmbH) pp 1-9

[15]   Rottengruber H, Wiebicke U, Woschni G et al 1999 Investigation of a Direct Injecting Hydrogen Diesel-Engine *World Hydrogen Conf. XII. Buenos Aires* pp 1255–64

[16]   Rottengruber H, Wiebicke U, Woschni G et al 2000 Wasserstoff-Dieselmotor mit Direkteinspritzung, hoher Leistungsdichte und geringer Abgasemission. Teil 3: *Versuche und Berechnungen am Motor* /MTZ No 2 pp 122–8

[17]   Kavtaradze R, Zeilinger K and Zitzler G 2005 Ignition Delay in a Diesel Engine Utilizing Different Fuels. *High Temperature* vol 43 No 6 pp 951-60

[18]   Kavtaradze R Z, Natriashvili T M and Zelentsov A A 2015 Ignition Delay and Emission of the Noxious Substances in Double-Fuel Engines Working on the natural Gas and Syngases Chapter 15 (p. 109-20) in the Book: *Innovative Methods for Improvement of Technical, Economic and Ecological Efficiency of Motor Cars* (New-York: NOVA-Publishers) p 138

[19]   Kavtaradze R Z 2016 Improving the Ecological Indices of a Hydrogen Diesel Engine with Direct Gaseous Hydrogen Injection *Journal of Machinery Manufacture and Reliability* vol 45 No 4 pp 307–15