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Mechanics

Ecological Characteristics of the Direct Injection Hydrogen Diesel with the Use of the 3D Model

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Solution of the system of differential equations with partial derivatives is realized with the use of the numerical method of finite differences and 3D CRFD code AVL FIRE. In the form of verified 3D mathematical model an instrument is created, use of which at conversion of serial internal combustion engines working on the traditional oil fuel into working on the hydrogen, is especially important because with its help: values of local non-stationary temperatures are determined and on the basis of these temperatures local concentrations of nitric oxides in the engine cylinder (when T > 1700 K, according to thermal mechanism of Zeldovich, NO_x is generated); the values of the engine controllable (law, duration and angle of advance of the hydrogen injection) and constructional parameters (degree of compression, burning chamber form, design of the inlet collector and injector) are ascertained that ensure minimization of NO_x. It is also ascertained that velocities of the burning process and heat release in the cylinder, dynamics of generation of the nitric oxides, values and redistribution of their local concentrations for the hydrogen and traditional diesels, essentially differ from each other that can be explained by the unique thermo-physical properties of hydrogen as the engine fuel. On the basis of results of the carried out numerical experiments we conclude that the use of the developed and verified 3D mathematical model significantly decreases material expenses and the time spent on designing and creation of the diesel engine with direct injection of the gaseous hydrogen. *© 2020 Bull. Georg. Natl. Acad. Sci.*

Hydrogen diesel, modeling, nitrogen oxides

The diesel engines stand out from the existent heat-engines by the highest efficiency. Therefore, their replacement by the more perfect alternative energy source is excluded in the nearest future. The alternative fuels, especially hydrogen, is the real way of solution of energetic and ecological problems posed before modern civilization.

The unique properties of hydrogen, as the engine fuel, stpulated development of two concepts: the petrol and diesel engines where hydrogen is used as a little additive to the traditional fuel (so called two-fuel engine) and the engine working on the hydrogen only with forced ignition. In this latter the hydrogen can be in the gasous (Daimler-Benz, Mazda, Ford, Toyota) or liquid phase (BMW 750HL).

Different concept – hydrogen diesel with direct injection of the gas hydrogen into the cylinder and self-ignition of the generated mixrure, is considered in the paper. The obvious advantages of this concept are: high efficience (the low fuel consumption), lack of detonation, possibility of the high super-charge, excellent ecology (CH, CO, CO_2 and soot are not emitted). Out of the harmful components restrected by the law the hydrogen diesel exhaust gases contain only one – nitric oxides NO_x. Besides, such engine does not an expensive cryogenic technology that is necessary for the case of liquid hydrogen.

Short Description of the Mathematical Model

It should be noted that the researches into hydrogen diesel carried out till today are mainly of experimental character, because of which consideration and analysis of possible conceptual and design variants are limited in the course of researches. This, of course, complicates generalization of the experimentally obtained results for diesels of other types and narrows the range of their utilization. Consequently, it is convenient to carry out prediction of the hydrogen diesel ecological and effective indices, study and analysis of influence of various constructional and controllable factors on these indices with the help of mathematical modeling of the thermo-physical processes proceeding in the cylinder.

The process of modeling implies: 1. Solution of the system of fundamental equations of momentum (Navier-Stokes), energy (Fourier-Kirchhoff), diffusion (Fick) and conservation of mass (continuity) with the help of the numerical method (method of controlling volumes); 2. Averaging of the mentioned system of equations by method of Favre at the initial stage and their writing in the form of Reynolds; 3. Addition of equations describing the turbulency, the hydrogen burning process and a mechanism of generation of the nitric oxides in this process, to this system.

The fundamental equations can be written in the form of generalized law of conservation of the substance according to which the sum of the non-stationary and convective flows is equal to the sum of the diffusion and source flows [1]:

$$\frac{\partial}{\partial \tau}(\rho\Phi) + div(\rho\vec{W}\Phi) = div(\Gamma_\Phi grasd\Phi) + S_\Phi, \tag{1}$$

where ρ is density, $\vec{W}$ – velocity vector, Φ – arbitrary independent variable, Γ_Φ – exchange (diffusion) coefficient, S_Φ – the term that can be presented as difference of flows of generation $S_{\Phi g}$ and annihilation $S_{\Phi a}$, or $S_\Phi = S_{\Phi g} - S_{\Phi a}$. A concrete form of Γ_Φ and S_Φ as well as $S_{\Phi g}$ and $S_{\Phi a}$ depends on essence of Φ [1, 2] and by substitution of corresponding values from equations (1) fundamental equations of momentum, energy, diffusion and conservation of mass (continuity) are obtained.

High-temperature reactions of the hydrogen oxidation are characterized by the scales of time that are of much shorter duration in comparison with the scales of time of the transfer processes. An approved burning model of Magnussen-Hjertager [2] is used in our case, which implies that burning of the air and hydrogen mixture proceeds simultaneously and therefore the average burning speed is determined by the time of turbulent mixing of the reagents.

Modeling of generation of the nitric oxides is based on the thermal mechanism of the nitric oxidation that is known by the name of expanded mechanism of Zeldovich [2]:

$$N_2 + O \underset{k_{1R}}{\overset{k_{1V}}{\leftrightarrow}} NO + N\,,\quad N + O_2 \underset{k_{2R}}{\overset{k_{2V}}{\leftrightarrow}} NO + O\,,\quad N + OH \underset{k_{3R}}{\overset{k_{3V}}{\leftrightarrow}} NO + H\,. \tag{2}$$

In these expressions k_i *(i=1, 2, 3)* denotes the speed constant of the corresponding reaction and subscripts *V* and *R* – direct and inverse reactions respectively. Dependence of the chemical reactions speed constants on the temperature is determined on the basis of Arrhenius' law [2, 3]. Replacement of the expanded mechanism of Zeldovich (2) by the so-called detailed mechanisms, when number of intermediate reaction, rises significantly (it reaches several hundreds), complicates the problem of selection of constants of the direct and inverse reactions speeds.

Comparative calculations of the nitric oxides concentrations (at various constants of kinetic reactions) are given in the work [4]. In our case, the more precise, approached to the experimental data values of concetration of NO in the hydrogen diesel are obtained with the use values offered by J. Warnatz and others [2] and H. Rottengruber [4] for direct and inverse reactions respectively. In all cases, speed constants of the kinetic reactions must be made more precise by comparison of the nitric oxides concentration obtained by modeling with the experimental data [2, 5, 6].

It is obvious that for studying of the nitric oxides generation in the hydrogen diesel burning chamber it is, first of all, necessary to carry out modeling of the non-stationary local temperatures in the cylinder local zones. These temperatures play decisive role not only in prediction of the hydrogen diesel ecologic indices but also in estimation of the local thermal loads on the engine basic details and their thermal stresses.

As it was mentioned earlier, Navier-Stokes' method of averaging equations, the so-called RANS (Reynolds-Averaged Navier-Stokes) method is used in our case and for closing the obtained system – k-ζ-f hybrid model of turbulency offered and realized by professor K. Hanjalic and others [7]. The advantage of this model is that the calculations can be carried out at any distance $y^+ \overset{def}{=} \frac{y}{\nu}\sqrt{\frac{\tau_w}{\rho}}$ practically from the wall (τ_w is friction stress, ν – kinetic viscosity, ρ – density). The model of turbulence k-ζ-f is in fact an improved, widely used lately model of turbulence of P. A. Durbin [8] that considers anisotropy of the near-wall turbulence.

A semi-implicit method SIMPLER (Semi-Implicit Method for Pressure-Linked Equations-Revised) [9] was used for numerical solution of the system of equations (1) of transfer that is developed for stage-by-stage calculation of type Predictor-Corrector. The numerical experiments were carried out with the use of the 3D CRFD code AVL FIRE [9].

It should be noted that for modeling the processes proceeding in the burning chamber of hydrogen engines they used traditional methods, based on the equations of thermo-dynamics [4], without considering the turbulence till today.

The Results of Modeling of Working Processes in the Traditional and Hydrogen Diesels

An indicator diagram or variation of the pressure in the cylinder with time (with the angle of rotation of the crank-shaft) as well as changes of the average temperature and heat release velocity are obtained by modeling. These parameters were studied on both, the base and the converted to hydrogen modifications.

Technical data of the high-speed, four-cycle, v-shaped, six-cylinder engine, converted to hydrogen engine with air supercharge and intermediate cooling of the supercharging air are: cylinder diameter/piston stroke D/S=130/140 mm/mm; the engine effective power Ne=315 KW at frequency of rotation n=2000 s^{-1}, degree of compression ε=16.5; burning chamber is located in the piston.

The volume of the engine cylinder that is confined by the immobile (cylinder head and shaft) as well as mobile (piston and valves) surfaces, is defined by the laws of movement of the crank-slider and valve

driving mechanisms. A calculate of the working process local parameters – temperature, density, speed etc., in realized for this variable volume.

The preliminary verification of the developed 3D mathematical model was realized by comparison of the calculated indicator diagrams with experimental diagrams obtained on the one-cylinder hydrogen diesel created on the base of MAN 24/30 [4, 5, 10] or diagrams obtained by models OD (by the program AVL BOOST) approved in the theory of internal combustion engines.

Studying the hydrogen engine working process, for its comparison with the traditional (base) diesel, the hydrogen cyclic feeding is determined from the condition $m_{ds}/m_{H2}=H_{ds}/H_{H2}$, where m_{ds} is the cyclic feeding of the diesel fuel. In our case H_{ds}=42.9 MJ/kg and H_{H2}=120 MJ/kg are respectively the least heat capacities of the diesel and hydrogen fuels. At satisfaction of the noted condition indicator diagrams of the traditional and hydrogen diesels coincide with each other and the values of the cycle maximum pressure are identic – P_Z=16 MPa.

It should be noted that hydrogen is characterized by significantly small time of the self-ignition delay. It is possible to control speed of the heat release and hence speed of the pressure rise by prolongation of the period of the hydrogen feeding in the engine cylinder. As a result of this, it becomes possible to avoid overly high values of P_Z that has a positive influence on basic details of the hydrogen diesel.

On the other hand, with the increase of the hydrogen burning duration the time interval increases, during which the heat absorbing surfaces of the burning chamber are under action of the high-temperature gases. This promotes rise of the thermal loads on the basic details forming the burning chamber volume [11, 12].

The burning processes of the air-fuel mixture in the hydrogen and traditional diesels are different. This is clearly seen at the change of the working body average temperature in the burning chamber volume with the angle of rotation of the crankshaft. Maximum value of the temperature in the traditional diesel cylinder is 1500 K and it approaches 1700 K in the hydrogen diesel. It should be noted that it is impossible to estimate content of NO_X in the burning products by the average volumic values of temperatures of the compared cycles [13].

Modeling of the Process of Generation of Nitrite Oxides at Burning of the Hydrogen

The reliable prediction of emission of the nitrite oxides can be realized only on the base of the working body local parameters, first af all those local non-stationary temperatures that are generated in the burning chamber at burning process of the hydrogen. Under the action of these temperatures (when their values excced 1700 k) oxidation of the nitrogen existent in the air takes place according to expanded mechanism of Zeldovich (2). The instantaneous local concentrations of local temperatures and nitric oxides of the working body in the hydrogen diesel cylinder obtained as a result of numerical integration of the system of differential equations of the transfer are given in Fig. 1 and Fig. 2 that confirm full correlation between the changes of the local temperature and local concentration of NO_X.

It should also be noted that the non-stationary local values of the temperature as values of the other local parameters (density, pressure and speed) of the working body are stipulated by the kinetic energy local values of turbulency in the turbulent processes of the flow and burning that depend significantly on the geometric form and sizes of the burning chamber. Such dependence is ascertained for both, the converted on the gas diesels with spark ignition [14] and traditional diesels [1], but for hydrogen diesels it is not studied till today.

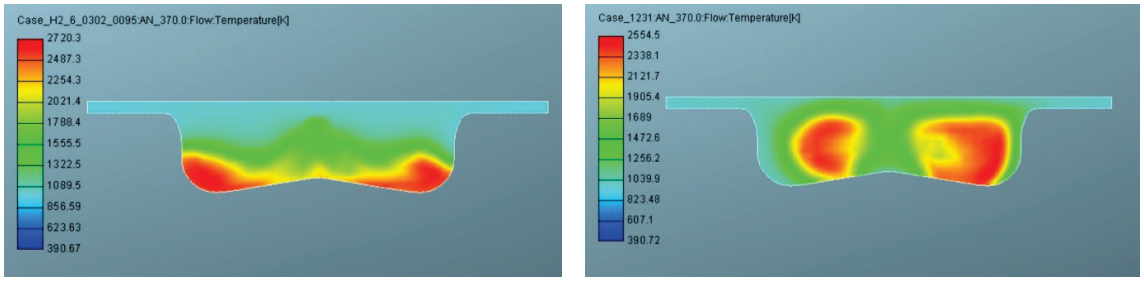

Fig. 1. The instantaneous local values of the temperature (K) in the burning chamber of the hydrogen (on the left) and traditional (on the right) diesels, when the angle of rotation of the crank-shaft $\varphi=370^0$ ($m_{ds}=0.24$ g/cycle, $m_{H2}=0.085$ g/cycle).

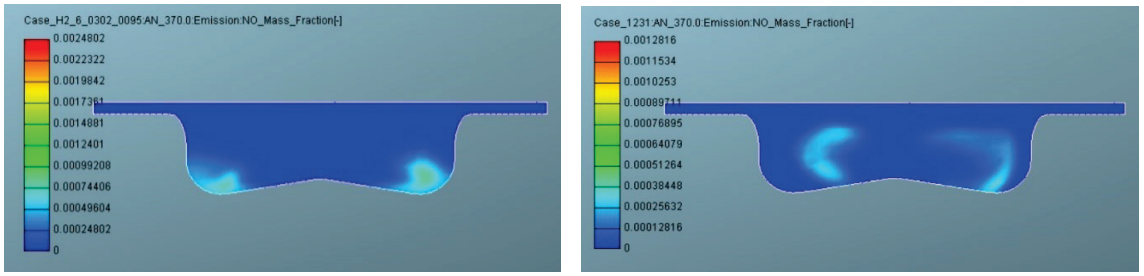

Fig. 2. The instantaneous local values of the nitric oxides concentrations (mass portion) in the burning chamber of the hydrogen (on the left) and traditional (on the right) diesels, when the angle of rotation of the crank-shaft $\varphi=370^0$ ($m_{ds}=0.24$ g/cycle, $m_{H2}=0.085$ g/cycle).

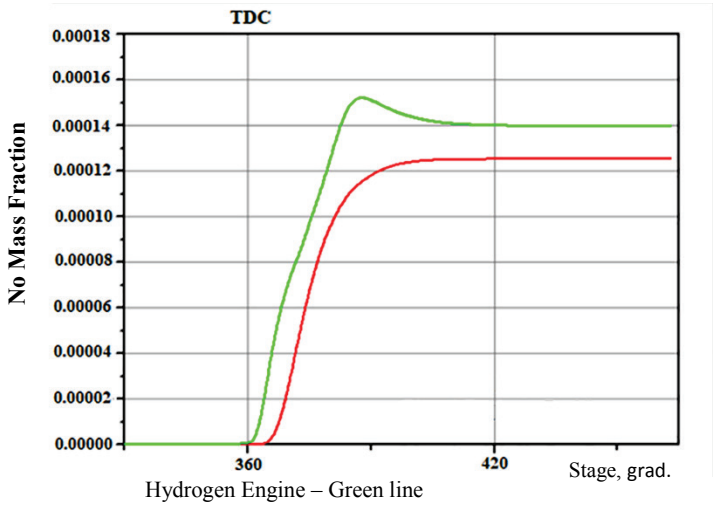

Fig. 3. Change of the nitric oxides total concentration depending on the angle of rotation of the crankshaft in the hydrogen (1) and traditional (2) diesels.

The results of modeling of processes of the nitric oxides generation in the burning chambers of the hydrogen and traditional diesels are shown in Fig. 3. The values of concentrations (mass portion) of the nitric oxides given here correspond to the concentration of the nitric oxides generated in the cylinder during the engine working cycle and are obtained by summation of local values of concentrations in the cylinder (Fig. 2). As it is seen, with increase of the local temperatures during the burning process the concentration of the nitric oxides rises according to mechanism of Zeldovich. After the temperature and correspondingly

NO_x reach their maximum values this concentration practically no longer changes (Fig. 3), despite the fact that the process of expansion proceeds in the cylinder and the temperature falls abruptly or the so-called „hardening“ of the nitric oxides takes place [1, 2].

The relatively increased values of the nitric oxides in the hydrogen diesel (Fig. 3) are explained by the high values of the local temperatures. To decrease these values it is necessary to use such approved methods as: decrease of the fuel injection advance angle, modification of the burning chamber form, change of the charge turbulence intensity in the process of inlet, change of the cyclic feeding and use of the multiple injection during the cycle [6, 10, 11].

Therefore, measures of decrease of the nitric oxides emission must, first of all, be directed towards decrease of the local temperatures in the hydrogen diesel burning chamber.

Conclusions. The results of the carried out researches allow us to make the following conclusions:
An instrument is created in the form of the developed 3D mathematical model with the use of which prediction and minimization of the nitric oxides concentration in the exhaust gases of the diesel with direct injection of the gaseous hydrogen are possible. It is ascertained by the numerical experiment that emission of the nitric oxides generated during the working process of the hydrogen diesel, when the cyclic dozes of the hydrogen and diesel fuel are selected considering their lowest thermal capacity ($m_{ds}/m_{H2}= H_{ds}/H_{H2}$=idem), exceeds by 10_15 % the similar index of the traditional diesel. It is possible to reduce emission of the nitric oxides even more (approximately down to the level of Euro-6 requirements) without installation of the neutralizers in the engine outlet system.

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მექანიკა

უშუალო შეფრქვევის წყალბადის დიზელის ეკოლოგიური მახასიათებლები 3D მოდელის გამოყენებით

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კერძო წარმოებულებიანი დიფერენციალური განტოლებების სისტემის ამოხსნა ხორციელდება სასრული სხვაობების რიცხვითი მეთოდისა და 3D CRFD კოდის AVL FIRE-ის გამოყენებით. ვერიფიცირებული 3D მათემატიკური მოდელის სახით შექმნილია ინსტრუმენტი, რომლის გამოყენებასაც განსაკუთრებული მნიშვნელობა ენიჭება ტრადიციულ, ნავთობური წარმოშობის საწვავზე მომუშავე სერიული შიგაწვის ძრავების წყალბადზე კონვერტირებისას, რადგან მისი საშუალებით: განისაზღვრება ლოკალური არასტაციონარული ტემპერატურების მნიშვნელობები; ამ ტემპერატურების საფუძველზე კი ძრავას ცილინდრში (როცა T > 1700 K, ზელდოვიჩის თერმული მექანიზმის თანახმად წარმოიშობა NOx) აზოტის ჟანგეულების ლოკალური კონცენტრაციები; დგინდება ძრავას რეგულირებადი (წყალბადის შეფრქვევის კანონი, ხანგრძლივობა და წინსწრების კუთხე) და კონსტრუქციული (კუმშვის ხარისხი, წვის კამერის ფორმა, შემშვები კოლექტორისა და ფრქვევანას კონსტრუქცია) პარამეტრების მნიშვნელობები, რომლებიც NOx-ის მინიმიზაციას უზრუნველყოფს. ასევე, დადგენილია, რომ ცილინდრის მოცულობაში წვის პროცესისა და სითბოს გამოყოფის სიჩქარეები, აზოტის ჟანგეულების წარმოქმნის დინამიკა, მათი ლოკალური კონცენტრაციების სიდიდეები და გადანაწილება, წყალბადისა და ტრადიციული დიზელების შემთხვევაში პრინციპულად განსხვავდება ერთმანეთისგან, რაც წყალბადის, როგორც ძრავას საწვავის უნიკალური თბოფიზიკური თვისებებით აიხსნება. ჩატარებული რიცხვითი ექსპერიმენტების შედეგების მიხედვით ვასკვნით, რომ დამუშავებული და ვერიფიცირებული 3D მათემატიკური მოდელის გამოყენება, აირადი წყალბადის უშუალო შეფრქვევის დიზელის ძრავას პროექტირებასა და შექმნაზე გაწეულ მატერიალურ დანახარჯებსა და ვადებს მნიშვნელოვნად ამცირებს, რაც მიღებული შედეგების გამოყენების მნიშვნელობაზე მიუთითებს.

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