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MODELLING OF PROCESSES OF NITROGEN OXIDES FORMATION IN CYLINDERS OF DIESEL ENGINES

Abstract

It is noted the presence of two groups of toxic components in diesels exhaust gases (EG): incomplete fuel combustion products and those of complete oxidation of the chemical elements in the fuel composition. The most numerous constituents of second category are the nitrogen oxides (NO_x). The content of the latter is regulated by IMO regulations and maximum limits apply to environmental control areas.

About 42% of nitrogen oxides emissions in an atmosphere are from diesel engines operaing on transport and in various industries. 80-90% of diesel engines exhaust gases nitrogen oxides is the share of nitrogen monooxide NO and 10-20 % - of nitrogen dioxide. The share of others gaseous nitrogen oxides (N_2O, N_2O_2, N_2O_4, N_2O_5) in the exhausted gases is insignificantly little, therefore widely applied designation NO_x serves for a designation of a nitrogen monooxides and dioxides mix.

The analysis of the different processes of formation of nitrogen oxides (NO_x) in the cylinder of internal combustion engines is carried out. There are following processes distinguished: main – thermal, including the extended Zeldovich mechanism of nitric oxide formation of NO from atmospheric nitrogen in the high temperature zone of combustion immediately after the combustion; generation of "prompt" NO in the flame front; fuel nitrogen oxides formation as a result of the conversion of nitrogen contained in the light and gaseous fuel to the nitrogen oxide when burned; the formation of NO from nitrous oxide N_2O. For modeling of diesel engines nitrogen oxides formation process, the preference is given to a thermal mechanism.

Existing semiempirical models of NO_x formation have low accuracy and require additional configuration for specific applications. It is suggested to consider the possibility of applying statistical models of NO_x formation. It is performed statistical analysis of experimental data using regression analysis. Regression equations of the second order with various options of interaction factors were obtained. The best predictive qualities posess a second order model with a nonlinear conversion function and cross-factor interaction, included in the model.

In article it is analysed modern representations about the mechanism of nitrogen oxides formation, making the basic part of harmful emissions with the exhaust gases of diesel engines. Essential components of this process are considered: thermal, "prompt", fuel, N_2O mechanisms. At calculation of nitrogen oxides formation the preference is given to a thermal variant. Insufficient accuracy of existing semiempirical models is noted and the expediency of the statistical approach on the basis of processing experimental data is proving.

Initial data for the statistical analysis are prepared. Regression dependences of speed of nitrogen oxides formation are received from defining parameters. Comparison of results of stochastic modelling for various structures of the equations is given. The best predicted properties posess the models on the basis of nonlinear transformation of criterion function.

Introduction. The merchant marine fleet is a basis of a global infrastructure of economic; it was and remains the most important type of transport for realization of the international exchange by the goods with the lowest influence on an environment and low costs for ton-mile of a transported cargo.

According to data of international conference UNCTAD (UNITED NATIONS CONFERENCE ON TRADE AND DEVELOPMENT) during period 2017 - 2030 expected mid-annual growth of sea transportations will make 3 - 4 % [19, p.16, Table 1.11].

At ship power installations (SPI) operation, the main and auxiliary diesel exhaust gases (EG) in an atmosphere are thrown out. The toxicity of EG by a grade of fuel and conditions of its combustionis is defined.

One of the tasks in solving the problem of improving the environmental performance of the SPI is the study and modelling of formation mechanism of nitrogen oxides in the cylinders of diesel engines.

The basic EG toxic components formed in SPI, by the nature of their occurrence can be divided on two basic groups. Products of incomplete combustion of fuel concern to the first group (carbon monoxide, hydrocarbons, aldehydes, soot). Toxic components of the second group - oxides of nitrogen NO_x and sulfur SO_x are formed as a result of full oxidation of the chemical elements which are a part of fuel and air [6].

The basic toxic component of SPI exhaust gases without dependence from type, dimensions and design features are nitrogen oxides NO_x. They are formed in the combustion chamber of a diesel engine, a gas turbine or a boiler furnace by oxidation of the nitrogen containing in air, and also nitrogen from nitrogenated molecules of fuel. NO_x share in total toxic emissions makes 30-80 % on weight and 60-95 % on equivalent toxicity. [5; 10, стр19-21].

On figure1 IMO requirements to ship diesel engines NOx emissiones are presented.

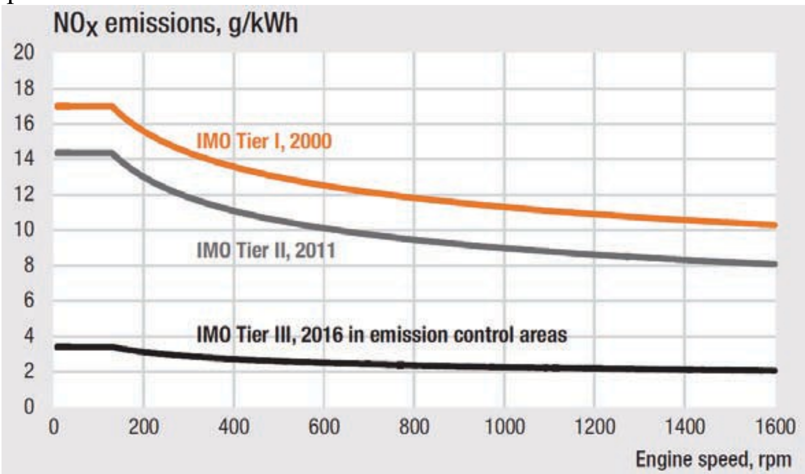

Fig.1. IMO requirements to ship diesel engines NO_x emissiones according to Marpol Annex VI [15, p. 162].

About 42 % of nitrogen oxides emissions in an atmosphere are from diesel engines working on transport and in various industries 80-90 % of diesel engines exhaust gases nitrogen oxides is the share of nitrogen monooxide NO and 10-20 % - of nitrogen dioxide. The share of others gaseous nitrogen oxides (N_2O, N_2O_2, N_2O_4, N_2O_5) in the exhausted gases is insignificantly little, therefore widely applied designation NOx serves for a designation of a nitrogen monooxides and dioxides mix. Nitrogen monooxide is an astable component. In an atmosphere under normal conditions nitrogen monooxide NO is oxidized up to dioxide NO_2 during 0,5 ÷100 hours depending on concentration in air [2].

Mechanisms of formation NO_x in SPI, thermal nitrogen oxides.

J.B.Zeldovich [3, p. 36] substantiated thermal character of the mecha-

$$O + N_2 \leftrightarrow NO + N - 196500J;$$

$$N + O_2 \leftrightarrow NO + O + 16720J.$$

nism of formation nitrogen oxide NO from atmospheric nitrogen in a zone of high-temperature burning and right after end of burning when rise in temperature leads to dissociation of molecular oxygen.At growth of temperature, since 2000K, speed of NO formation (direct reaction) increases very quickly (exponential dependence). It is visible, that the first reaction goes with absorption of a plenty of thermal energy.

Most often in calculations is expanded J.B. Zeldovich [3, стр.75] mechanism - in accordance with addition on D.L.Baulch [11] and G.A.Lavoi [18] reactions.

$$N + OH \leftrightarrow NO + H$$

It is used the semiempirical equation offered by D.B. Heywood [16, p. 575] for speed of formation of nitrogenoxides, being power function of temperature.

$$\frac{d[NO]}{dt} = \frac{6\times 10^{16}}{T^{1/2}} \exp\left(\frac{-69,090}{T}\right) \cdot [O_2]_e^{1/2} \cdot [N_2]_e \ \text{mole/cm}^3 \cdot \text{s}.$$

Here [NO] – nitrogenoxide concentration, [O_2], [N_2] - equilibrium concentration of oxygen and nitrogen at current pressure and temperature.

Zeldovich's thermal mechanism now is most in detail studied of all known mechanisms of nitrogen oxides formation. Nevertheless, in Z.R.Kavtaradze's opinion [4, p.66], at usage for calculations of nitrogen oxides formation in combustion chambers of piston engines there is a danger of reception of the inexact results, connected with errors of experimental definition or an unsuccessful choice of available constants of reactions speeds from references [4, p. 67].

The similar conclusion is received by us at processing skilled data F. Lin [12, fig 4-6, 4-9, 4-12 and 4-14] and H.P. Liu [17].

"Prompt" nitrogen oxides (Fast NO). The mechanism of formation "prompt" NO in front of a flame essentially differs from those for thermal NO and for the first time is described by C.P. Fenimore [13]. In the further this process was studied by C.K. Westbrook and F.L. Dryer at methanol burning [22].

Reaction has more complex character, as it is closely connected with formation of radical CH (in front of a flame) in conditions of a rich fuel-air mix.

$$CH + N_2 \leftrightarrow HCN + N;$$

$$N + OH \leftrightarrow NO + H;$$

$$N + O_2 \leftrightarrow NO + O.$$

The main thing in this mechanism - fast formation of atoms N. Speed of nitrogen oxide formation is defined by speed of reaction between intermediate radical CH and a molecule of nitrogen N_2 [20, p.19]. Reaction begins at temperature 800 K and does not depend almost on its further growth. As a result HCN (hydrocianic acid) is generated. This enters reaction with radical N - as a result NO forms very quickly. In diesel engines the share of “prompt” NO among all emissions NO_x is rather insignificant and makes less than 5 % [1, p. 6, 7; 16, p. 574], through small size of depth of front of a flame in combustion chamber conditions of a diesel engine (0,1мм) [16, p. 572], at rotation frequency n = 1000 rev/min) and the small period of time (for example, τ = =10÷50 μs or φ = 0,1÷0,3° crankshaft rotation angle (CRA) for front of a flame passage and CH radicals existence [1, p.6, 7].

Fuel nitrogen oxides. Transformation of the nitrogen, containing in light and gaseous fuel, in nitrogenoxides at combustion in transport diesel engines practically does not play a role, as fuel for these engines, in opinion Kavtaradze Z.R and Kavtaradze R.Z. [4, p. 68], almost does not contain some the connected nitrogen. Some other approach to fuel nitrogenoxides contains in A.S.Loskutova's and G.A.Weisser [8; 21, стр.38, 39] dissertational works - as usual, in fuel, used in ship diesel engines, the contents of nitrogen does not exceed 0,1 %, that can give NO contents up to 10 % [21, p. 39], but in calculations fuel NO are not considered in connection with the big difference in the contents of nitrogen in heavy fuels, received from oil from various deposits on different oil refineries.

Formation NO from N_2O. Nitrous oxide N_2O - causes formation nitrogenoxides NO in the event depleted fuel-air mix limits radical CH formation, blocking occurrence "prompt" NO, and insignificant further growth of temperature interferes with formation thermal NO [1, p.6,7].

As a whole, many authors [1, p. 6, 7, 35; 4, p. 67, 68; 7; 8; 9; 16, p. 572, 574, 577; 21, p. 39] consider, that for calculations of quantity NO_x (including usage one-, two -, and multi-zone models of combustion chamber), formed at burning in diesel engines at work in a nominal mode, and a choice of a technique of their reduction it is necessary to use the thermal mechanism. The share of "prompt", fuel and NO, formed on N_2O mechanism, usually makes 5÷10 %, that does not exceed size of an error at use of the thermal mechanism.

The basic contents. Considering stated, it is expedient at research of processes of nitrogen oxides formation in cylinders of diesel engines to use the tools of statistical representation of the regularities of the phenomenon under study .

With this purpose in this paper the analysis of experimental data obtained in the studies of Fangfang Lin [12] is carried out. Used graphs of Fig.4-6, Fig and Fig 4-12 4-14 source, combined in the form of preoriginally introduced in Fig. 2. On the chart plotted the values of average temperature in the cylinder and the NO content for the two variant of data on the composition of the air charge: 21% and 34% of the recirculated exhaust gas (EGR).

The average temperature in the cylinder is determined by calculation according to the pressure measured with the Kistler sensor.

The NO_x concentration was measured at the outlet of the cylinder, and intermediate values were determined by calculation. The agreement between the calculated and experimental values was marked sufficient for practical purposes.

The experiment was carried out on the engine with a common rail direct fuel injection system. The main parameters of the engine: cylinder diameter - 96 mm; piston stroke - 105 mm; compression ratio - 14.3; rotation frequency - 1200 rpm, the charged air pressure - 0.14 MPa; mean indicated pressure 0.8 MPa.

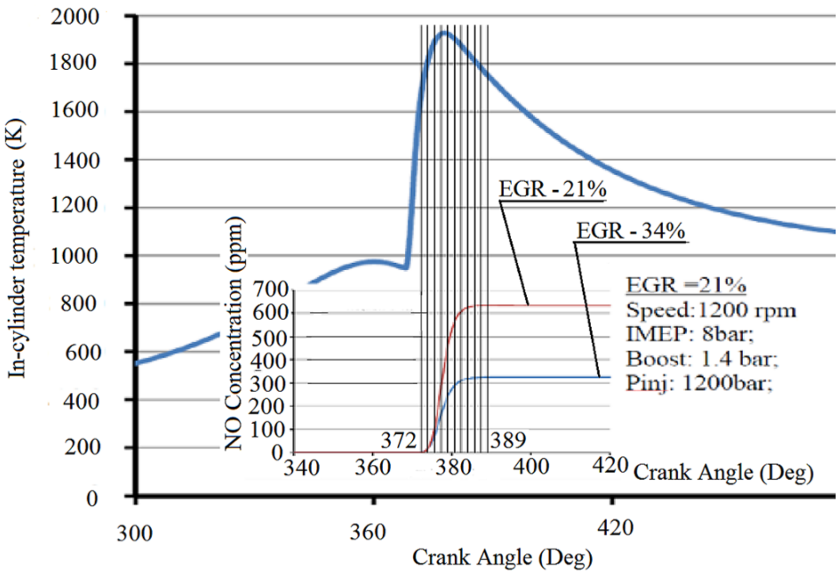

Fig.2. Formation of nitrogen oxides in the diesel engine cylinder

Used in value analysis of the NO content in the exhaust gas is equal to 1200 ppm, obtained by extrapolation of the dependence of this parameter from the level of the EG recirculation. The period of NO formation was 372º ÷ 389º crankshaft rotation angle (CRA).

In the preparation of statistical processing of experimental data, the objective was to obtain the dependence of the current rate of formation of NO from the following conditions of reaction: temperature, pressure, nitrogen concentration, oxygen concentration. To calculate the current values of these parameters used geometric data of the engine, state information of the air charge, given in view of a course of reaction of NO formation

The ultimate goal of the analysis was to obtain the objective function VNO=f (T, R, VO_2, VN_2) as a polynomial in the framework of multiple regression analysis using software package STATISTICA.

Along with the above Fangfang Lin data [12] are used the results of Zhixia He [14].

To set the parameters of the statistical processing two tables are composed: one for the initial phase of the process –to the maximum reaction rate (table 1) and the second for the period of speed reduction (table 2).

In tables the following symbolic notation and dimensions are used:

VNO - current rate of formation of NO, g/ ($cm^3 \cdot s$) 10^{-3},

T - average temperature in the cylinder , 10^2 K,

P - gas pressure in cylinder, bar,

VN_2 – current concentration of N_2, mg/cm^3,

VO_2 - current O_2 concentration, mg/cm^3.

Line numbering takes into account source of data: the initial part refers to F. Lin [12], the second section - Z. He [14].

Table1.The initial section of raw data for multiple regression analysis

№	VNO	T	P	VN_2	VO_2
1	0	11	112	65	19.8
2	13.309	13.5	135	66	18.9
3	16.258	14.5	142	65	17.9
4	21.028	15.5	143	64	16.6
5	21.472	16.7	144.5	62	15.2
6	25.142	17	143.5	60	13.7
1	0	16.3	77	25.5	7.2
2	3.69	18	81.19	24.4	6.91
3	24.06	19	81.47	23.2	6.13
4	44.28	19.2	78.05	22	5.4

As mentioned above the actual analysis was carried out separately for the data of each table (tab.1, tab.2) using the technique of polynomial regression of second order STATISTICA with and without taking into account the effects of cross-factor interaction of the first order between the factors T-P, T-VO_2, P-VN_2.

Table 2. The second section of the initial data for multiple regression analysis

№	VNO	T	P	VN_2	VO_2
7	19.202	17.4	140	57	12.3
8	9.056	17.45	132.5	54	10.8
9	6.318	17.5	127.2	51	9.4
10	4.78	17.6	120	48	8.2
11	4.072	17.35	112.5	44	6.9
12	3.088	17.25	106	41	5.8
13	0.936	17	98	38	4.8
14	0.596	16.75	88	35	4
5	34.77	19.3	74.32	20.8	4.72
6	25.57	19.1	69.54	19.7	4.09
7	8.03	18.9	64.91	18.5	3.16
8	1.8	18.5	59.94	17.5	2.98
9	1.49	18.1	55.29	16.5	2.49
10	0.65	17.9	51.54	15.6	2.06
11	0.5	17.5	47.53	14.7	1.66

Thus, processing without the use of a nonlinear transformation consists of four areas of analysis:

1-table.1, the VNO to the maximum value without accounting for cross-factor interaction,

2-table.1, the VNO to the maximum value taking into account cross-factor interaction,

3-table.2, after VNO maximum values without taking into account cross-factor interaction,

4-table.2, VNO after the maximum value taking into account cross-factor interaction.

Additionally performed analysis using nonlinear transformations separately for each table.

In the record of the results obtained in STATISTICA, the original transcription of the character symbols and table design. In particular, the exponentiation indicated by “T^2”. For each option the basic statistics of the obtained regression equations are displayed in tabular form. In the article they are given selectively.

Table 3. Statistics of the regression equations of VNO of the second order (section1)

Slave Variable	SS of model & SS of residuals (Up to max)										
	Multiple R	Multiple R2	Corrected R2	SS Model	Dgr. of freedom Model	MS Model	SS Residual	Dgr. of freedom Residual	MS Residual	F	p
VNO	0.99993	0.99986	0.99877	1665.60	8	208.200	0.22756	1	0.22756	914.908	0.02556

Table 4. Additional statistics regression VNO equations of the second order (section1)

Effect	Univariate significance tests for VNO (Up to max) Sigma restricted parameterization. Hypotheses decomposition				
	SS	Degrees of freedom	MS	F	p
Free term	11.77066	1	11.77066	51.72463	0.087954
T	2.16208	1	2.16208	9.50099	0.199716
T^2	2.86442	1	2.86442	12.58733	0.174900
P	4.42014	1	4.42014	19.42370	0.142044
P^2	6.52554	1	6.52554	28.67564	0.118252
"VN_2”	2.23240	1	2.23240	9.81000	0.196744
"VN_2”^2	6.44429	1	6.44429	28.31858	0.118252
"VO_2”	19.34972	1	19.34972	85.02982	0/068770
"VO_2”^2	2.09603	1	2.09603	9.21073	0.202633
Err	0.22756	1	0.22756		

Section 1. As a result of table. 1 data processing regression equation of the second order, irrespective of cross-factor interaction at the site of growth of the VNO is obtained. Table. 3, 4 and 5 contain the statistical characteristics of the obtained equation.

The predicted equation for VNO to a maximum value without accounting for cross-factor interactions (section 1) is received in the form of:

VNO=597.672916-22.825184*T+.667768144*T^2-2.6786585*P +.012566513*P^2-7.1092035*"VN_2" + .130309987 * "VN_2" ^2-27.384921 * "VO_2" + .430460105 * "VO

Table 5. Additional statistics regression VNO equations of the second order (section1)

Effect	Estimators of parameters (Up to max) Sigma-restricted parameterization									
	VNO Param.	VNO Std. Err	VNO t	VNO p	-95% Conf. int.	+95% Conf. int.	VNO Beta	VNO Std. Err^2	-95% Conf. int.	+95% Conf. int.
Free term	597.6729	83.10265	7.19198	0.087954	-458.246	1653.592				
T	-22.8252	7.40508	-3.08233	0.199716	-116.916	71.265	-4.2781	1.387939	-21.9136	13.35730
T^2	0.6678	0.18833	3.54786	0.174900	-1.724	3.059	3.8507	1.085355	-9.9400	17.64143
P	-2.6787	0.60779	-4.40723	0.142044	-10.401	5.044	-6.1096	1.386265	-23.7238	11.50460
P^2	0.0126	0.00235	5.35496	0.117530	-0.017	0.042	6.3605	1.187779	-8.7316	21.45267
"VN_2"	-7.1092	2.26979	-3.13209	0.196744	-35.950	21.731	-10.8097	3.451285	-54.6625	33.04299
"VN_2" ^2	0.1303	0.02449	5.32152	0.118252	-0.181	0.441	17.3882	3.267533	-24.1297	58.90619
"VO_2"	-27.3849	2.96979	-9.22116	0.068770	-65.120	10.350	-11.5927	1.257188	-27.5668	4.38136
"VO_2" ^2	0.4305	0.14184	3.03492	0.202633	-1.372	2.233	4.5133	1.487138	-14.3825	23.40922

In the tables the following symbolic notations are used .

R2 - coefficient of determination -is an indicator of the degree of fit of the model to the data;

R=√R2— coefficient of multiple correlation is also an estimate of the prediction quality;

Adjusted R2 is the adjusted R2 taking into account the number of parameters in the regression equation.

SS-sum of squares of the observed values , adjusted for average;

F – Fisher criterion;

p, (p-level) is the significance level;

Beta – standardized regression coefficients (weights) of the Beta value allows us to compare the contributions of each predictor in the prediction of response;

Dgr.of Fr – degree of freedom

MS - mean square – sum of squares due to difference of average between groups.

Further, in Fig. 3 the comparison of the observed and predicted values VNO is given.

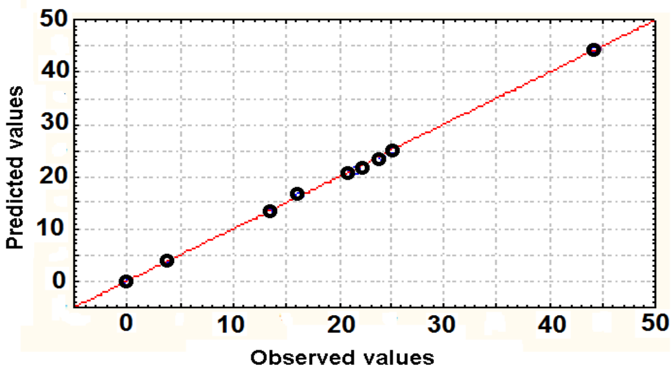

Fig. 3. The observed and predicted values for the analysis of the VNO up to the maximum

Section 2. VNO up to the maximal value (Tab.1) in view of interfactorial interaction.

The predicted equation for:

VNO=-481.19017-64.754350*T+5.54908884*T^2+.291158320*P-.00655917*P^2+58.2186552 * "VN_2"-.54820820 * "VN_2" ^2-39.234503

* "VO_2"-2.6052584 * "VO_2" ^2-1.0250779*T*P +.479690167*T * "VN_2" + .821523252*P * "VO_2"

Static characteristics of the obtained models are close to the parameters presented in the first section, and without loss of information content can be omitted.

Section 3. After VNO maximum values (Tab.2) excluding cross-factor interaction.

Predicted equation:

VNO=2443.13559-271.31367*T+7.83224882*T^2-9.3893914*P +.051233660*P^2+19.7223414*"VN_2"-.32924052*"VN_2"^2+ 10.7479560* "VO_2"+ .327007343*"VO_2"^2

The parameters of the regression equation remain close to the first sector does not contain significant additional information and are omitted here.

Sector 4. After VNO maximum values (Tab.2) given the cross-factor interaction. Predicted equation:

VNO=2957.66525-311.90138*T+8.92817160*T^2-21.488015*P +.103951466*P^2+30.6109206 * "VN2"-.19515754 * "VN2" ^2 + 60.5761228 * "VO2" + 4.73294512 * "VO2" ^2 +.429225399*T*P-.91203859*T* "VN2"-1.1361444*P * "VO2".

The above considerations on the statistics of the model are stored and in the fourth sector.

Table 6. Combined table with a non-linear transformation up to the maximum VNO

№	Log VNO	VNO	T	P	VN_2	VO_2
1	-7	0	11	112	65	19.8
2	1.124145425	13.309	13.5	135	66	18.9
3	1.211067119	16.258	14.5	142	65	17.9
4	1.322797968	21.028	15.5	143	64	16.6
5	1.331872498	21.472	16.7	144.5	62	15.2
6	1.400399822	25.142	17	143.5	60	13.7
1	-7	0	16.3	77	25.5	7.2
2	0.567026366	3.69	18	81.19	24.4	6.91
3	1.381295623	24.06	19	81.47	23.2	6.13
4	1.646207612	44.28	19.2	78.05	22	5.4

We consider next the regression results with the preliminary transformation (logarithm) function (VNO). Similarly used the above approach deals with two areas: from minimum to maximum values (tab.6) and the other values on the section of decreasing values (table. 11). The analysis is performed in the package STATISTICA. The resulting regression equation (second order) with subsequent potentiation. We also consider the option given the cross-factor interaction.

The equation for the predicted increase in Log VNO excluding cross-factor interaction is obtained in the form of:

"Log_VNO"=-166.71463+8.22083786*T-.20298448*T^2 +2.11672513*P-.00831373*P^2-1.1636426 * "VN_2" + .009908180 * "VN_2" ^2-2.1415420 * "VO_2" + .094858083 * "VO_2" ^2.

Statistics of the presented equation are given in tables.7,8,9. For other variants of the analysis these parameters are close here again and are omitted here.

Table 7. Statistics of the equation of increase Log VNO excluding cross-factor interaction

Effect	Univariate significance tests for Log VNO (Log power 2)				
	SS	Degrees of freedom	MS	F	p
Free term	0.915843	1	0.915843	0.527129	0.600211
T	0.280463	1	0.280463	0.161425	0.756787
T^2	0.264674	1	0.264674	0.152238	0.763101
P	2.760132	1	2.760132	1.588641	0.426979
P^2	2.856137	1	2.856137	1.643899	0.421691
"VN_2”	0.059809	1	0.059809	0.034424	0.883211
"VN_2”^2	0.037257	1	0.037257	0.021444	0.907433
"VO_2”	0.118333	1	0.118333	0.068108	0.837482
"VO_2”^2	0.101784	1	0.101784	0.058584	0.848820
Err	1.737416	1	1.737416		

Table 8. Additional statistics of the equation of increase Log VNO excluding cross-factor interaction

Effect	Estimators of parameters (Log power 2 up) Sigma reststricted parametrization									
	LogVNO Param.	LogVNO Std. err.	LogVNO t	LogVNO p	-95.00% Conf. int.	+95.00% Conf. int.	LogVNO Beta	LogVNO Std. err.^{2}	-95.00% Conf. int.	+95.00 % Conf. int.
Free term	-166.71	229.62	-0.7260	0.6002	-3084.3	2750.9				
T	8.221	20.461	0.4017	0.75678	-251.76	268.20	6.0087	14.9552	-184.01	196.03
T^2	-0.203	0.5203	-0.3903	0.76310	-6.81	6.405	-4.5646	11.6948	-153.16	144.03
P	2.113	1.6794	1.2604	0.42697	-19.22	23.455	18.827	14.9372	-170.96	208.62
P^2	-0.008	0.0065	-1.2821	0.42169	-0.09	0.074	-16.410	12.7985	-179.03	146.21
"VN_2"	-1.164	6.2717	-0.1855	0.88321	-80.85	78.526	-6.8998	37.1881	-479.42	465.62
"VN_2"^2	0.010	0.0677	0.1464	0.90743	-0.85	0.870	5.1558	35.2082	-442.21	452.52
"VO_2"	-2.142	8.2059	-0.2609	0.83748	-106.4	102.12	-3.5353	13.5464	-175.65	168.59
"VO_2" ^2	0.095	0.3919	0.2420	0.84882	-4.89	5.075	3.8785	16.0241	-199.72	207.48

Table 9. Additional statistics of the equation of increase Log VNO excluding cross-factor interaction

Depend. Variable	SS of residuals & SS of models (Log power 2 up)										
	Multiple R	Multiple R2	Correct. R2	SS Model	Dgr.of freedom Model	MS Model	SS Residual	Dgr.of freedom Residual	MS Resid-ual	F	p
Log VNO	0.99203	0.98413	0.85727	107.81	8	13.476	1.7374	1	1.7374	7.7561	0.2712

Obtained data allow to judge efficiency of nonlinear transformation and inclusion in model cross-factor interaction. With this purpose it is made table10 where corresponding data are included.

Apparently, the account of cross-factor interaction (CFI) improves result considerably.

Table 10. Comparative characteristics of models

№	VNO init.	VNO-CFI	VNO+CFI
1	0	0	0
2	13.309	19.127	13.309
3	16.258	10.768	16.258
4	21.028	21.176	21.028
5	21.472	34.899	21.472
6	25.142	17.556	25.142
1	0	0	0
2	3.69	0.61	3.69
3	24.06	176.016	24.06
4	44.28	18.164	44.28

The analysis of values after maximum LogVNO with preliminary non-linear transformation of function is executed, as it was specified above, according to tab. 11.

The analysis after maximal value VNO excluding cross-factor interaction.

The predicted equation for LogVNO on a reduction sector excluding cross-factor interaction looks like:

"Log_VNO"=40.1114431-5.0719228*T+.160720080*T^2-.13451155*P+ .001041513*P^2 +.304140170 * "VN_2"-.00604247 * "VN_2" ^2-.04479961 * "VO_2" + .013469301 * "VO_2" ^2

For the same data including cross-factor interaction the next expression is received

"Log_VNO"=286.562574-34.380169*T+.990499970*T^2 +3.12711025* P-.00294767*P^2-7.1391513 * "VN_2"-.00931342 * "VN_2" ^2-2.6002619 * "VO_2"-.19598768 * "VO_2" ^2-.15707391*T*P +.417142157*T * "VN_2" + .058530257*P * "VO_2"

Table 11. The combined table after VNO maximum

№	Log_VNO	VNO	T	P	VN_2	VO_2
7	1.283346465	19.202	17.4	140	57	12.3
8	0.956936414	9.056	17.45	132.5	54	10.8
9	0.800579622	6.318	17.5	127.2	51	9.4
10	0.679427897	4.78	17.6	120	48	8.2
11	0.609807769	4.072	17.35	112.5	44	6.9
12	0.489677292	3.088	17.25	106	41	5.8
13	-0.028724151	0.936	17	98	38	4.8
14	-0.22475374	0.596	16.75	88	35	4
5	1.541204691	34.77	19.3	74.32	20.8	4.72
6	1.407730728	25.57	19.1	69.54	19.7	4.09
7	0.904715545	8.03	18.9	64.91	18.5	3.16
8	0.255272505	1.8	18.5	59.94	17.5	2.98
9	0.173186268	1.49	18.1	55.29	16.5	2.49
10	-0.187086643	0.65	17.9	51.54	15.6	2.06
11	-0.301029996	0.5	17.5	47.53	14.7	1.66

Table 12.Comparative characteristics of models

№	VNO	VNO-CFI	VNO+CFI
7	19.202	19.605	20.232
8	9.056	7.93	7.427
9	6.318	7.563	7.608
10	4.78	5.033	5.167
11	4.072	3.624	3.877
12	3.088	2.482	2.275
13	0.936	1.215	1.23
14	0.596	0.571	0.576
5	34.77	44.293	42.194
6	25.57	17.429	18.139
7	8.03	7.438	7.596
8	1.8	2.659	2.672
9	1.49	1.135	1.232
10	0.65	0.782	0.669
11	0.5	0.458	0.485

Comparative table (tab.12) of VNO values after a maximum is indicative of less essential, than in the previous case, contribution of cross-factor interaction (CFI) in prognostic properties of stochastic model improvement.

Conclusions

The basic mechanism defining speed of nitrogen oxides formation in the diesel engines cylinder, thermal oxidation of nitrogen of air is.

Existing semiempirical models of this process demand individual adjustment and do not ensure reception of reliable results.

It is expedient to consider an opportunity of application for calculations of stochastic models on the basis of experimental data.

Statistical processing of an available experimental material with various variants of regression equations has revealed the best variant. It has appeared nonlinear transformation of criterion function including cross-factor interaction of independent variables.

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