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## Three-Way Catalyst Modeling For the Gas Engine.

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### ABSTRACT

Radical reduction of environmental pollution focuses on creating completely clean internal combustion engines. Neutralizing system development for such engine is based on the implementing of three-way catalytic converter units. A reliable estimation of the catalyst unit parameters significantly reduces experimental engine fine-tuning and configuration management system. This paper covers the process of modeling a catalyst for a diesel engine, converted for gas fuel. The implementation of a perfect neutralization system provides high ecologic standards. The estimated mathematical model allows to calculate the characteristics of a catalytic block in a wide range of parameters. The results from rather simple model describe the basic laws of flow, heat transfer and heterogeneous chemical kinetics occurring in the catalyst. The theoretical results were improved by experiments on a real engine.

**Keywords:** vehicle, gas engine, exhaust aftertreatment system, heterogeneous catalysis, mass transfer, heat transfer.

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## INTRODUCTION

Using engines operating on the attractive gas (methane) engine fuel is one of promising lines of development of internal combustion engines (Ipatov *et al.*, 2010; Luksho *et al.*, 2015; Panchishny *et al.*, 2015). The use of economically attractive motor fuel stimulates the sales of engines, which in turn compensates for the costs associated with the development of a new engine (Terenchenko *et al.*, 2015). However, the cost of developing a completely new engine is high, which hinders launching new projects in this direction. A more promising direction is the conversion of diesel engines with the preservation of basic structures, units and assemblies, the change of the working process parameters and adding the necessary systems. This makes it possible to significantly reduce the cost of the project.

One of the features of methane fuel consists in different combustion conditions, which, in particular, causes the need to change valve timing and operate on the Miller cycle. The use of the Miller cycle makes it possible to achieve high performance indicators. Modern engine control systems make it possible to monitor and ensure the optimal parameters of ICE systems, including the values of the stoichiometric coefficient, depending on the engine load and speed.

In the modern context, an essential requirement is the environmental safety of an ICE, especially of a newly developed one (Azarov and Kutenev, 2015). In this case, the most advanced requirements to the amount of emitted regulated toxic components are included in the initial technical design assignments for ICE. This makes it possible to streamline the work process so as to ensure the lowest possible emissions of toxic components CO, CO<sub>2</sub>, CH, NO<sub>x</sub> and particulate matter. For some modes of engine operation (idle and close to rated), in most cases it is impossible to ensure the required parameters of emissions only by the working process, and this leads to the need to use neutralization systems or exhaust gas aftertreatment systems (EGATS).

Despite the fact that in case of using methane fuel in the Miller cycle the toxicity parameters are relatively low, the use of EGATS is necessary. In this case, one of the most attractive and reasonable designs is the use of a three-way methane catalyst and an optional additional recovery module for nitrogen oxides (Panchishny, 2007; Panchishny *et al.*, 2015).

This article deals with the research of the exhaust gas aftertreatment system for a converted Miller-cycle diesel engine and a neutralization system built on the basis of a three-way catalyst.

To calculate the EGATS parameters, including those of a EGATS on the basis of three-way catalysts, a number of software systems can be used. The most common are BOOST systems, developed and supported by AVL List, and AXISuit systems by Exothermia. There are corresponding calculation units in the wide-spread CAD systems ANSYS and NX. The above-mentioned software systems deal with the calculation of the engine working processes and ensure obtaining the required characteristics of EGATS for the initial stage of design. The settings of software systems make it possible to change the parameters of a mathematical model, on the basis of which they are built, which provides the flexibility of routine calculations. However, significant changes of the built mathematical model are not possible. Therefore, for research purposes it is necessary to develop customized mathematical models, making it possible to take into account the determined dependencies and to analyze the functionality in a wide range of parameters. The presented study is based on the developed functional model of the kinetics of a catalytic reactor-converter.

Most modern EGATS and neutralization systems are based on the use of catalyst-coated ceramic blocks. As a rule, a ceramic block is made from cordierite, consists of a plurality of parallel channels (the channel size is about 0.001 m) with a porous wall (the diameter of pores is from 2 to 500 micrometres) with a developed surface (up to 5,000 m<sup>2</sup> per 1 m<sup>3</sup> of volume). Cell density is 300, 400, 600 and 900 cells per square inch or 46, 62, 93, 139 cells per square centimeter, respectively. The thickness of the applied catalytic layer is 50 micrometers. Exhaust gases after passing through the long and thin channels (the channel size/length ratio d/L is from 50 to 250) diffuse in the catalytic layer, are adsorbed by the catalyst molecules, interact and return (diffuse) into the flow of moving exhaust gases. An overview of current achievements in the development, application and designing of catalytic converters is presented in (Nadareishvili *et al.*, 2015).

There are a large number of works on the development of mathematical models of varying complexity and accuracy, aimed to describe processes in catalytic reactors (Koltakis *et al.*, 1997; Koci *et al.*, 2004; Chatterjee *et al.*, 2001; Kwon *et al.*, 2007; Koop *et al.*, 2009; Mladenov *et al.*, 2010; Oh and Cavendish, 1982; Koltakis *et al.*, 1997; Siemund *et al.*, 1996; Kim *et al.*, 2009; Voltz *et al.*, 1973; Montreuil *et al.*, 1992; Dubien *et al.*, 1998; Pontikakis *et al.*, 2001; Pontikakis *et al.*, 2004; Caroline *et al.*, 2013). The simplest models are presented in (Koltakis *et al.*, 1997). There are fairly complex mathematical models that take into account the vast majority of reactions in elementary forms (Koci *et al.*, 2004; Chatterjee *et al.*, 2001; Kwon *et al.*, 2007; Koop *et al.*, 2009; Mladenov *et al.*, 2010). Preparation and calculations by such models are cumbersome and require significant efforts. Therefore, most of the research is built on using common reactions without dividing into the elementary stages and the application of the Langmuir-Hinshelwood principle (Oh and Cavendish, 1982; Koltakis *et al.*, 1997; Siemund *et al.*, 1996; Kim *et al.*, 2009). This approach is built on the work (Voltz *et al.*, 1973), which was the first to study the kinetics of the oxidation of CO and C<sub>3</sub>H<sub>6</sub>. However, NO was excluded from the examination.

A great number of experimental studies of various designs on the basis of three-way units were conducted. However, these data cannot be used directly in the design purposes. In practice, the results of the tests can't be recalculated into the parameters of reactions taking place in the catalyst.

One of the first works describing the configuration of the parameters of chemical kinetics is (Montreuil *et al.*, 1992). A large number of conversion coefficients for CO, NO, C<sub>3</sub>H<sub>8</sub>, C<sub>3</sub>H<sub>6</sub>, H<sub>2</sub>, O<sub>2</sub> were obtained.

In (Dubien *et al.*, 1998), the technique of determining the preexponential factor and activation energy was proposed.

In (Pontikakis *et al.*, 2001), the behaviour of an exhaust neutralization system was analyzed. A 2D model for the thermal state of the block and a change of 12 kinetic parameters were used. A similar approach was applied in (Pontikakis *et al.*, 2004). In (Caroline *et al.*, 2013), a very simplified model was described.

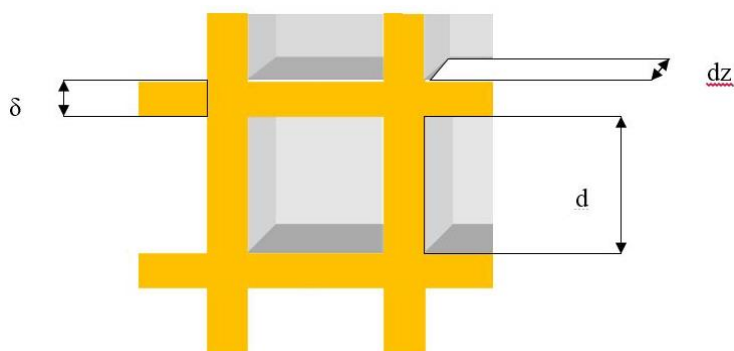


Figure 1. Simulation model of a single channel of a catalytic unit

## RESEARCH METHODS

The research method applied in the article is based on the theoretical parametric study with the analysis of the obtained results using the data of a test of a real natural gas fueled engine in the range of stoichiometric ratio of 0.9-1.1.

## RESULTS AND DISCUSSION

The mathematical model described in this paper is based on the complete system of equations describing the state of the system “flow – boundary layers – a layer of catalyst” for a single channel, Figure 1. The mutual influence of channels is minimal; it is enough to consider the impact of the environment.

The mathematical formulation of the thermal problem takes the form of a system of differential equations (Nadareishvili, 2015):

Energy equation for the flow

$$\rho * c_p * \left( \frac{\partial T}{\partial \tau} + v \frac{\partial T}{\partial x} + u \frac{\partial T}{\partial y} + w \frac{\partial T}{\partial z} \right) = \frac{\partial}{\partial x} \left( \lambda \frac{\partial v}{\partial x} \right) + \frac{\partial}{\partial y} \left[ \lambda \left( \frac{\partial T}{\partial y} \right) \right] + \frac{\partial}{\partial z} \left[ \lambda \left( \frac{\partial T}{\partial z} \right) \right] + q_v + \alpha_{wall} (T_{wall} - T_{gas}) \quad (1)$$

Energy equation for the body of the block

$$\frac{\partial}{\partial x} \left( \lambda_c \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left[ \lambda_c \left( \frac{\partial T}{\partial y} \right) \right] + \frac{\partial}{\partial z} \left[ \lambda_c \left( \frac{\partial T}{\partial z} \right) \right] = \alpha_{wall} (T_{gas} - T_{wall}) + \alpha_{inner} (T_{inner} - T_{gas}) + q_v \quad (2)$$

where  $\rho$  kg/m<sup>3</sup>,  $c_p$  J/(kg · K<sup>0</sup>),  $\lambda$  W/(m · K),  $\mu$  Pa/s are density, specific heat capacity at constant pressure, thermal conductivity and viscosity of exhaust gases;  $\lambda_{wall}$  W/m · K<sup>0</sup> is thermal conductivity of a block wall;  $\alpha_{wall}$  W/(m<sup>2</sup> · K<sup>0</sup>) is the heat transfer coefficient of a channel wall; P Pa is pressure;  $T_{inner}$ ,  $T_{gas}$ ,  $T_{wall}$  K<sup>0</sup> are the temperatures of ambient air, exhaust gases and separation wall; V, U, W, m/s are speed components,  $q_v$  W/m<sup>3</sup> is the density of spatial sources of the heat of chemical reactions.

In general terms, the flow in a channel of a catalyst is described by the unsteady-state Navier-Stokes equation (3-5) and the mass-transfer equation (6).

Navier-Stokes equation

$$\rho * \left( \frac{\partial v}{\partial \tau} + v \frac{\partial v}{\partial x} + u \frac{\partial v}{\partial y} + w \frac{\partial v}{\partial z} \right) = \rho g_x \frac{\partial p}{\partial x} + \frac{\partial}{\partial x} \left( 2\mu \frac{\partial v}{\partial x} - \frac{2}{3} \mu \text{div}V \right) + \frac{\partial}{\partial y} \left[ \mu \left( \frac{\partial v}{\partial y} + \frac{\partial u}{\partial x} \right) \right] + \frac{\partial}{\partial z} \left[ \mu \left( \frac{\partial v}{\partial z} + \frac{\partial w}{\partial x} \right) \right] \quad (3)$$

$$\rho * \left( \frac{\partial u}{\partial \tau} + v \frac{\partial u}{\partial x} + u \frac{\partial u}{\partial y} + w \frac{\partial u}{\partial z} \right) = \rho g_y \frac{\partial p}{\partial y} + \frac{\partial}{\partial y} \left( 2\mu \frac{\partial u}{\partial y} - \frac{2}{3} \mu \text{div}V \right) + \frac{\partial}{\partial x} \left[ \mu \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) \right] + \frac{\partial}{\partial z} \left[ \mu \left( \frac{\partial u}{\partial z} + \frac{\partial w}{\partial y} \right) \right] \quad (4)$$

$$\rho * \left( \frac{\partial w}{\partial \tau} + v \frac{\partial w}{\partial x} + u \frac{\partial w}{\partial y} + w \frac{\partial w}{\partial z} \right) = \rho g_z \frac{\partial p}{\partial z} + \frac{\partial}{\partial z} \left( 2\mu \frac{\partial w}{\partial z} - \frac{2}{3} \mu \text{div}V \right) + \frac{\partial}{\partial x} \left[ \mu \left( \frac{\partial w}{\partial x} + \frac{\partial w}{\partial z} \right) \right] + \frac{\partial}{\partial y} \left[ \mu \left( \frac{\partial w}{\partial y} + \frac{\partial w}{\partial z} \right) \right] \quad (5)$$

where  $\rho$ ,  $c_p$ ,  $\lambda$ ,  $\mu$  are density, specific heat capacity at constant pressure, thermal conductivity and viscosity of exhaust gases; P is pressure;  $g_x$ ,  $g_y$ ,  $g_z$  m/s<sup>2</sup> are components of bulk forces; V, U, W are components of velocity.

For the flow, the mass-conservation equation (mass-transfer equation) is written in the form of the distribution of the concentration of the substance in the flow of exhaust gases in the channel for each component:

$$\frac{\partial C}{\partial \tau} + v \frac{\partial C}{\partial x} + u \frac{\partial C}{\partial y} + w \frac{\partial C}{\partial z} = D_m \left( \frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2} \right) - r \quad (6)$$

where  $D_m$  m<sup>2</sup>/s is the molecular diffusion coefficient;  $r$  mol/(m<sup>3</sup> · s) is the invariant rate of a chemical reaction.

The equation of the distribution of the concentration of the substance on the boundary porous layer

$$\frac{\partial C}{\partial \tau} = D_m \left( \frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2} \right) - r \quad (7)$$

The equation of the distribution of the concentration of the substance on the active porous layer

$$\frac{\partial C}{\partial \tau} = -r \quad (8)$$

The energy equations, written for the flow and the body of the catalytic unit, can be changed by adopting the quasi-stationary nature of the process, the smallness of the heat transfer by thermal conductivity along the flow in the direction of x, y, z in relation to convection transfer, fully developed flow (U = W = 0), low rate of chemical reactions (the absence of homogeneous reactions) in the flow.

Then the energy equations will be as follows:

For the flow

$$\rho * c_p * v \frac{\partial T}{\partial x} = \alpha_{wall} (T_{wall} - T_{gas}) \quad (9)$$

For the unit

$$\frac{\partial}{\partial x} \left( \lambda_{wall} \frac{\partial v}{\partial x} \right) = \alpha_{wall} (T_{gas} - T_{wall}) + \alpha_{inner} (T_{inner} - T_{gas}) + q_v \quad (10)$$

At  $u = w \approx 0$  as compared to  $v$ , the effects of longitudinal and transverse mixing can be neglected. The processes of longitudinal diffusion, the rate of which is less than the rate of the linear mass transfer, can also be neglected in the equation; therefore, the summand  $D_m \frac{\partial^2 C}{\partial z^2}$  tends to zero, and  $\frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2}$  is regarded as a superposition of two identical flows in one direction.

Then the mass-transfer equations for the  $i$ -th component in the flow without regard for homogeneous reactions are as follows:

$$v \frac{\partial C}{\partial x} = 2D_m \frac{\partial^2 C}{\partial y^2} \quad (11)$$

$$\frac{\partial C}{\partial x} = 2 \frac{D_m}{v} \frac{\partial^2 C}{\partial y^2}, \quad (12)$$

where  $V$  is the flow rate;  $\frac{\partial^2 C}{\partial y^2}$  – is the driving force

The diffusion coefficient for the  $i$ -th component is determined by the Fuller-Schettler-Giddings formula depending on temperature

$$D_m = D_0 \left( \frac{T}{T_0} \right)^{1.75} \quad (13)$$

Effective diffusion coefficient

$$D_{eff} = \frac{\varepsilon}{\frac{1}{D} + \frac{1}{D_k}} \quad (14)$$

where  $\varepsilon = \frac{v_p}{v_{cat}}$  is the porosity ratio;

$D_k$  is the diffusion coefficient, calculated according to the Knudsen formula, taking into account the diffusion in narrow pores

$$D_k = \frac{d_p}{3} \sqrt{\frac{8RT}{\pi M}} \quad (15)$$

where  $d_p$  m is the pore diameter;

$M$  mol/kg is the molecular weight of the  $i$ -th component

Let us determine the value of  $C_s$  – the surface concentration of the  $i$ -th substance on the catalyst. According to the Langmuir-Hinshelwood mechanism:

$$r = \frac{\partial C}{\partial t} = k\theta_i\theta_j \quad (16)$$

or, in quasi-stationary approximation

$$C = k\theta_i\theta_j \quad (17)$$

$$\text{where } \theta = \frac{k_{ad}A_i}{1+k_{ad}A_i} \quad (18)$$

$\theta_i$  is the fractional covering,  $k_{ad}$  is the adsorption equilibrium constant,  $A_i$  is the number of active adsorbing centers.

The impact of the catalyst is taken into account as a correction factor of activation energy for the catalytic reactor:

$$\text{If, } F = \frac{E_{cat}}{E} < 1 \quad (20)$$

where  $E_{cat}$  is the activation energy in the presence of a catalyst, and  $E$  is the standard activation energy of the reaction.

Then

$$k = k_0 e^{\frac{-FE}{RT}} \quad (21)$$

where  $k_0$  m<sup>3</sup>/mol is the preexponential coefficient;

$E$  J/mol is the activation energy;

$R$  J/(mol \* K<sup>0</sup>) is the universal gas constant.

As a result, the system of equations (1)-(10) is transformed as follows  
For an elementary section  $\Delta z$ :

For the flow

$$v \frac{\partial v}{\partial z} = -\frac{1}{g} (P_{in} - P_{out}) \quad (22)$$

$$\varepsilon v \frac{\partial C}{\partial z} = D_m 4d (C_{gas} - C_{wall}) \quad (23)$$

$$\rho C_p v \frac{\partial T}{\partial z} = \alpha_w 4d (T_{gas} - T_{wall}) \quad (24)$$

For the body of the catalyst

$$(1 - \varepsilon) v \frac{\partial C}{\partial z} = -D_m \theta_i (C_{wall} - C_{gas}) - r_i \quad (25)$$

$$\rho C_p \frac{\partial^2 y}{\partial z^2} = \alpha_w 4d (T_{gas} - T_{wall}) - \alpha_{inner} \pi \frac{x D^2}{4} (T_{wall} - T_{inner}) - \Sigma \frac{\Delta h_i r_i}{M_i} \quad (26)$$

where  $4d$  m is the perimeter of the cell surface;

$D$  m is the diameter of the unit;

$\Delta h_i$  J/mol is the enthalpy of each elementary reaction;

$M_i$  is the molecular weight of the  $i$ -th component.

The reaction rate  $r_i$  in the active layer in the catalyst according to (17)

$$r_i = \frac{k_i C_1 * \dots * C_i}{u_i} \quad (27)$$

Boundary conditions

$$z = 0 \quad (28)$$

$$T_{gas} = T_0, T_{wall} = T_1, T_{inner} = T_2 \quad (29, 30, 31)$$

$$C_{iin} = C_{i0}, C_{iwall} = 0, \theta_i = 0 \quad (32, 33, 34)$$

Depending on temperature, exhaust gas parameters are determined by the following dependencies

$$\rho = 1 * 10^{-6}T^2 - 0.003T + 2.0218 \quad (35)$$

$$\mu = 3.49 * 10^{-8}T - 6.6539 * 10^{-6} \quad (36)$$

$$C_p = 0.28T + 966.12 \quad (37)$$

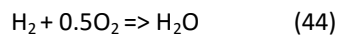
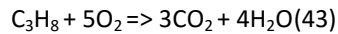
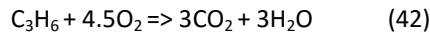
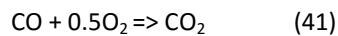
$$\lambda = 0.00158e^{0.0016T} \quad (38)$$

$$Pr = 0.76315e^{-0.00023T} \quad (39)$$

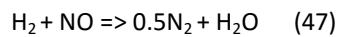
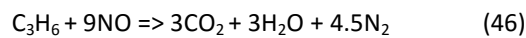
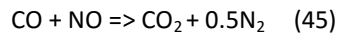
$$Sc = 0.90215e^{-0.00023T} \quad (40)$$

The main considered reactions in a three-way catalyst

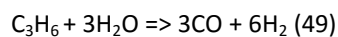
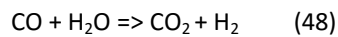
Oxidation reactions



NO reduction reaction



Water reforming



The reaction rates are determined as

$$r_i = K_i C_i C_{i+1} e^{-FE_i/RT} \quad (50)$$

The built model was numerically optimized in relation to unknown quantities. Preexponential coefficients and the values of activation energy are shown in Table 1.

**Table 1 – Preexponential coefficients and the values of activation energy**

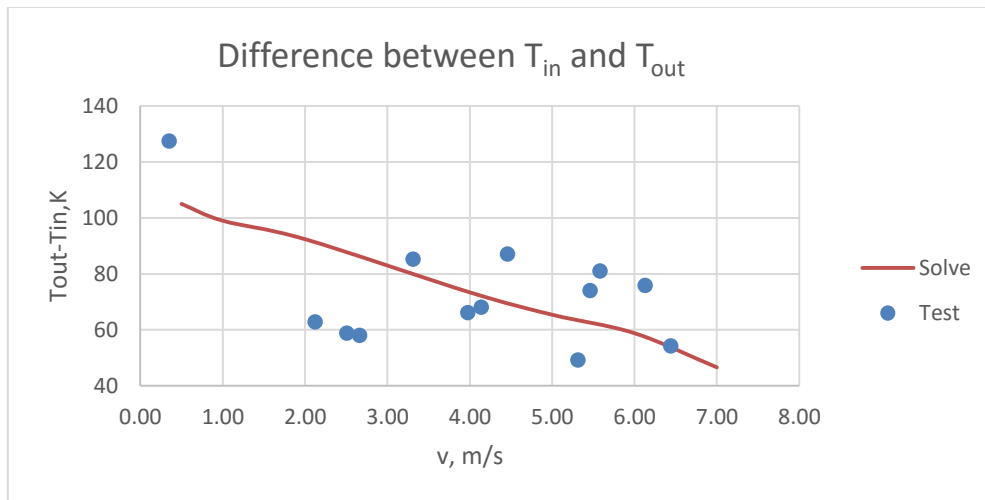
Reactions	$k_{0i}$	$FE_{i,r}$
$CO + 0.5O_2 \Rightarrow CO_2$	3.79E + 12	111450
$C_3H_6 + 4.5O_2 \Rightarrow 3CO_2 + 3H_2O$	1.02E + 14	129530
$C_3H_8 + 5O_2 \Rightarrow 3CO_2 + 4H_2O$	4.68E + 09	165160
$H_2 + 0.5O_2 \Rightarrow H_2O$	3.79E + 12	111450
$CO + NO \Rightarrow CO_2 + 0.5N_2$	1.61E + 14	52374
$C_3H_6 + 9NO \Rightarrow 3CO_2 + 3H_2O + 4.5N_2$	6.20E + 09	90063
$H_2 + NO \Rightarrow H_2O + 0.5N_2$	6.10E + 09	69237
$CO + H_2O \Rightarrow CO_2 + H_2$	1.80E + 05	56720
$C_3H_6 + 3H_2O \Rightarrow 3CO + 6H_2$	1.23E + 05	81920

For the verification of the obtained results, the authors used the test data for a methane-fueled engine with a three-way catalyst with the following characteristics, presented in Table 2.

**Table 2 – Parameters of a three-way catalyst of a methane-fueled engine**

Unit diameter, m	0.2286
Unit length, m	0.2023
Number of cells per square inch	300
Wall thickness, m	0.000165
Porosity	0.7
Metal loading, g/ft <sup>3</sup>	100
Formulation of the composition Pt Pd: Rd	0:14:1

The comparison of calculated and measured temperatures is presented in Figure 2.



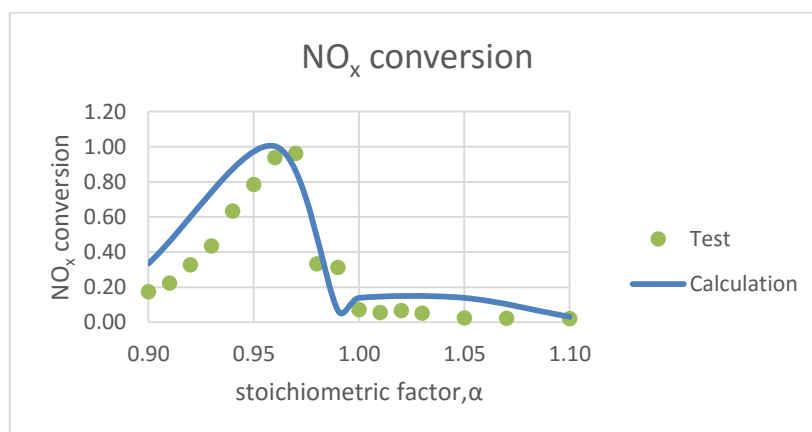
**Figure 2. Change of temperatures in the catalytic unit depending on flow rate**

The comparison was based on the overall temperature difference in the unit depending on the changes in the flow rate of exhaust gases. The above graph shows a sufficient consistency of results.

The tests were conducted with the change of the stoichiometric coefficient within the range from 0.9 to 1.1.

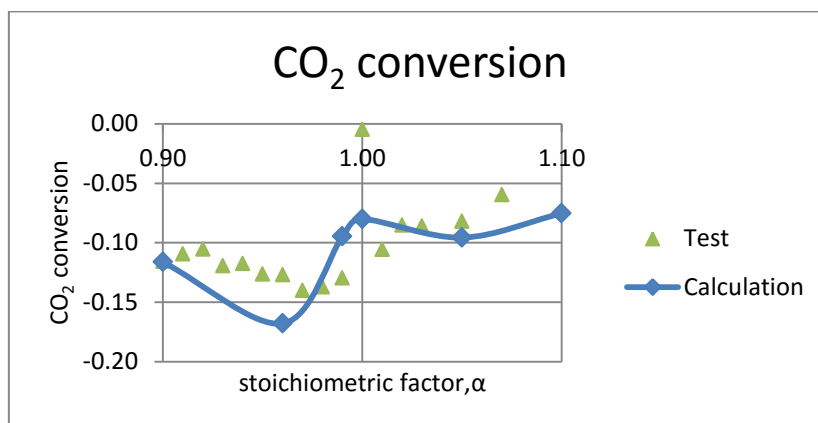
On the basis of the obtained results, conversion coefficients were calculated, which are determined as

$$CV = \frac{(C_{in} - C_{out})}{C_{in}}$$



**Figure 3. NO<sub>x</sub> conversion**




 Figure 4. CO<sub>2</sub> conversion

### CONCLUSIONS

The conducted theoretical research made it possible to build a mathematical model, substantiate the dimensionality (2D) and verify the results of the parametric study on real results. The developed model of a three-way catalytic unit for a natural gas fueled engine has a sufficient reliability and makes it possible to design neutralization systems in a wide range of input parameters.

The obtained results confirmed the significant impact of the flow rate in a converter channel within the range up to 8 m/s on the temperature of the flow and the catalytic layer, and consequently on the processes of diffusion and chemical kinetics. The dependence of NO<sub>x</sub> and CO<sub>2</sub> conversion on the stoichiometric ratio within the range of 0.9-1.1 was obtained.

### ACKNOWLEDGMENTS

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