Generalized Models of Processes Occurring in Neutralization Systems

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ABSTRACT

Reducing the toxicity of internal combustion engines is a competitive advantage compared to an electric transmission. The main tool is the development of post-treatment systems for treated gases. Reducing the cost of developing such systems consists in reducing experimental testing and increasing the volume of calculation work. Decision-making in determining the strategy for the conversion of toxic substances is based on a preliminary analysis of the initial system. A correctly formulated mathematical model allows analyzing the influence of design parameters (block diameter, temperature, and engine volume) on the efficiency of the system and the ability to achieve design parameters.
The article shows the process of constructing a mathematical model with the corresponding assumptions, its subsequent optimization and reduction to a generalized dimensionless form. The analysis of the influence of design parameters on gas-dynamic, thermal and physical-kinetic processes is carried out.

Key words: heat engine, ecology, post-treatment system, mathematical model.

1. INTRODUCTION
A system that effectively reduces the toxicity of exhaust gases from an internal combustion engine and has been developed over the past 30 years is a neutralization system. This is a system combining high efficiency and providing a reduction of 100% of the toxic components of CO, CH, NO and particulate matter to standardized levels recognized as safe, providing outstanding compactness, making it possible to place it on vehicles. The operation and astonishing efficiency of up to 99% of the conversion of the neutralization system are based on sophisticated complex aerodynamic, chemical, and thermal processes taking place in the core of the catalytic unit or catalyst system. The process of developing catalysts has reached perfection, but differs in complexity and depth [1,2].

The basis for the development of both the neutralization system and the core of the system – the catalytic unit – are processes that occur primarily on the developed surface of the channel of the catalytic unit [3].

From the beginning of consideration of the possibility of using catalysts in automotive neutralization systems, mathematical models of processes with different completeness were considered, in accordance with the goals set, which described the ongoing processes.

Objective of the research
This article is devoted to one of the approaches, based on the development of a generalized mathematical model of the catalyst and its analysis of relationships and mechanisms.

2. PROPOSED METHODOLOGY

2.1 General description
The first models were proposed in the 1970s; they were intended for an analytical solution, therefore they were simplified.
Further, with the development of computational numerical methods, the models became more complicated and described in more detail complex processes that occurred on the surface of the catalytic block of the layer.

Two features of the development of mathematical models should be noted. First of all, sophisticated, complex, developed mathematical models were not considered in a dimensionless form, since they were intended to be solved in a numerical form. It should be noted that such a solution allows getting a fairly accurate solution, but it is very demanding in terms of the specification of the initial and boundary conditions and is difficult to be analyzed and generalized.

Therefore, the second feature, especially at the present time, is the absence of simple, but effective models for quick analysis of processes and evaluation of the effectiveness of structures.

Let us consider the evolution of mathematical models described by the system of equations.
In sufficient detail, the development of mathematical description approaches in the last century from the 1960s was considered in [4].

One of the first models mentioned is the model [5]:

$$\varepsilon\rho c \frac{\partial T}{\partial t} + \frac{G}{A} c \frac{\partial T}{\partial x} = \frac{\partial}{\partial x}\left(\varepsilon k \frac{\partial T}{\partial x}\right) - hG(T_g - T_m). \qquad (1)$$

The model considers the behavior of the temperature of the exhaust gases and the surface of the catalyst under a number of assumptions (without taking into account the thermal conductivity of the catalyst monolith, the heat capacity of the block). In the models used by other authors [6-9], these assumptions were taken into account. A comparison of 1D and 2D calculations showed that 1D calculations were 10 times faster. Some models [10] considered a stationary solution that did not cause design difficulties.

In [8], concentrations instead of molar fractions were operated, in [11], solutions for block and flow temperatures were obtained independently, in [12], the influence of radiation on the formation of temperatures was taken into account, in [13], the model consisted of a set of pellets, the papers [14,15] were devoted to the consideration of radial heat conductivity in the block, in [16], the movement of masses on the catalytic surface was considered in the stationary case, in [17,18], the accumulation of oxygen by cerium was taken into account for the three-component catalyst, which significantly complicated the mathematical model, and the papers [19,20] took into account the work of active centers in kinetics.

The article [21] presents the calculations according to the following model:

$$\rho c \left(\frac{1}{\gamma} \frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} \right) = -\frac{hG}{\varepsilon} (T_g - T_m), \ (2)$$

$$\frac{\partial C}{\partial t} = \frac{kG}{1-\varepsilon} (C_g - C_s) - \frac{CR}{1-\varepsilon}. \ (3)$$

In [22, 23, 24], the calculation was carried out using the WAVE and GT-Power software products, which were developed for well-studied mathematical models.

In [25], the model consisted of seven differential equations. A model with real emission data was tested and an aging model for catalytic converters was proposed. In [26], a two-dimensional catalytic converter with 21 channels was simulated taking into account chemical reactions; the flow rate, velocities, and mass velocities were studied in order to evaluate the effect of the flow, which was unevenly distributed in the catalytic converter, on the conversion efficiency. In [27], the influence of the input temperature and the channel shape on the catalyst efficiency were considered.

The need for modern modeling was shown in [28] and approaches were proposed for the implementation of structural submodels for analyzing the processes of reducing toxic emissions of diesel engines.

It should be noted that of the listed works, only a small part [7] was devoted to the rigorous mathematical

formulation of aerodynamic, thermal, and catalytic processes in a dimensionless form. This is due to the fact that software solution methods based on the standard WAVE and GT-Power programs make it possible to solve specific one-dimensional and three-dimensional problems in a direct formulation. The development of hardware allows for detailed calculations at reasonable intervals and obtaining values suitable for calculating the design of neutralization systems and their catalytic units. However, it is very difficult to conduct a generalized analysis based on dimensional mathematical models, which is associated with a huge number of calculated options.

Therefore, consideration of models in a dimensionless form is preferable in most cases.

In all the models examined, the parameters are considered irrespective of the engine parameters and their relations. Such an approach does not allow evaluating the effectiveness of processes in relation to a specific class of engine and/or a specific engine [29-31].

In most cases, the models under consideration did not take into account the initial section of the flow and heat transfer, which does not allow taking into account the significant efficiency of the processes at maximum driving forces.

2.2 Algorithm

In this section, the proposed system of mathematical modeling of the processes of the neutralization system will be considered.
Let us consider in detail the physical and chemical model of the catalytic unit with an arbitrary section of the catalytic channel with some characteristics.

The exhaust gas mixture flows through the catalytic unit with the flow rate Q and temperature T and the concentration Ci of the i-th component.

The parameters of the catalytic unit (Figure 1,2,3) are as follows:
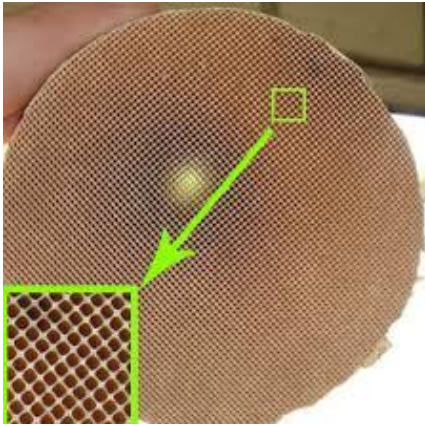
L is the length of the unit, meter;

D is the diameter (characteristic size) of the unit, meter;

d is the characteristic size of the unit cell of the unit;

δ is the unit cell wall thickness;

$Fb = \frac{\pi D^2}{4}$ is the unit cross-sectional area;

$d_j = 1/d^2$ is the number of cells per square meter of the unit for a square cell.

**Figure 1:** The structure of the ceramic block

Most modern neutralization systems (exhaust gas post-processing systems) are based on the use of ceramic blocks with a catalytic coating (Figure 2). A ceramic block is usually made of cordierite, consists of many parallel channels (channel size of about 0.001 m) with a porous wall (pore diameter from 2 to 500 micrometers) with a developed surface (up to 5,000 m^2 per m^3 of volume). The cell density is 300, 400, 600 and 900 cells per sq. inch or 46, 62, 93, 139 cells per cm^2, respectively. The thickness of the applied catalytic layer is 50 micrometers. Exhaust gases passing through long (the ratio of the channel size to the length, d/L, ranges from 100 to 500) thin channels diffuse into the catalytic layer, are adsorbed by the catalyst molecules, enter into interaction, and return (diffuse) back into the flow of moving exhaust gases.
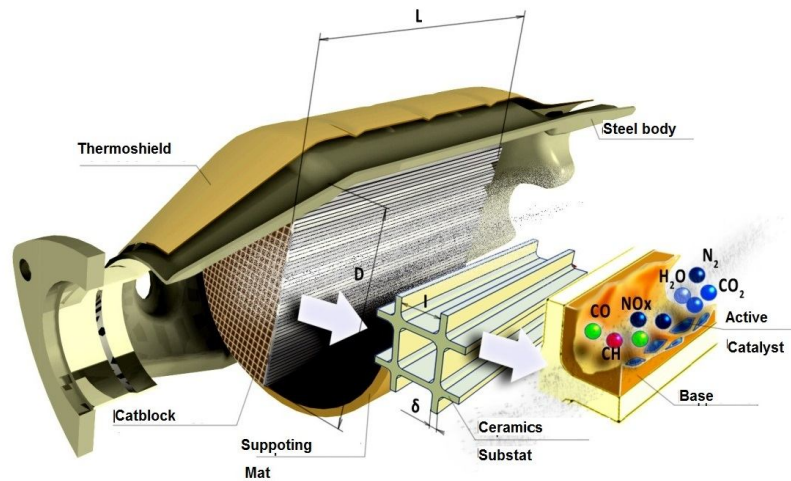
Figure 2: The design of the converter

First of all, let us consider replacing a catalytic unit with numerous channels with a unit with a single channel, the effective characteristics of which will be equivalent to the original unit.

The diagram of a single channel converter is shown in Figure 3.
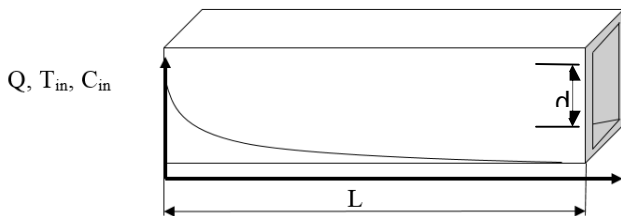
Figure 3: Single channel diagram

Key assumptions and estimates:

1. All channels are geometrically identical.

2. All channels are thermally identical in the absence of radial energy loss. It is possible to take into account the boundary effects for external channels when constructing the methodology for the general calculation of the catalytic block.

It follows from Assumptions 1 and 2 that the single-channel model describes the behavior of all channels in a block.

3. A simple channel shape is assumed. The authors consider the square shape, which is predominant, along with the triangular.

4. The processes are not developed, the length of the initial section is up to 20 calibers, and the total length of the channel is up to 500 calibers.

5. The reactions are catalytic, heterogeneous and, in some specified cases, homogeneous. Chemical reactions in the gas phase, as a rule, can be neglected, since the reaction rate at active centers is several orders of magnitude higher than the rate of unmotivated reactions.

From Assumption 5, part of the reaction of complex reactions can be neglected.

Under the assumptions made, a single channel can be considered as an ideal displacement reactor, consisting of successive ideal mixing reactors, and the entire catalytic unit – as ideal reactors operating in parallel.

2.3 Flow Chart

The motion scheme of the reacting substances is shown in Figure 4.
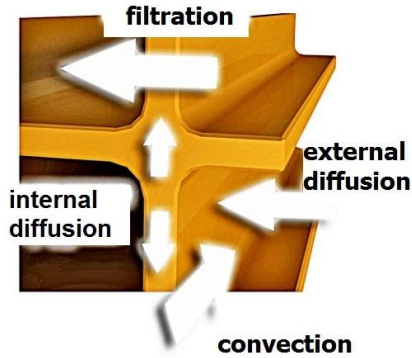
Figure 4: Motion scheme of the reacting substances

In general, the problem has the form of a system of differential equations:

The energy equation for flow is as follows:
$$\rho c_p\left(\frac{\partial T}{\partial \tau} + v\frac{\partial T}{\partial x} + u\frac{\partial T}{y} + w\frac{\partial T}{\partial z}\right) = \frac{\partial}{\partial x}\left(\lambda\frac{\partial v}{\partial x}\right) + \frac{\partial}{\partial y}\left[\lambda\left(\frac{\partial T}{\partial y}\right)\right] +$$
$$\frac{\partial}{\partial z}\left[\lambda\left(\frac{\partial T}{\partial z}\right)\right] + q_v + {} + \alpha_{wall}\left(T_{wall} - T_{gas}\right) \quad (4)$$

The energy equation for block array is as follows:

$$\frac{\partial T}{\partial \tau} - \frac{\partial}{\partial x}\left(\lambda_{wall}\frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left[\lambda_{wall}\left(\frac{\partial T}{\partial y}\right)\right] + \frac{\partial}{\partial z}\left[\lambda_{wall}\left(\frac{\partial T}{\partial z}\right)\right] =$$
$$\alpha_{wall}\left(T_{gas} - T_{wall}\right) + \alpha_{inner}\left(T_{inner} - T_{gas}\right) + q_v \quad (5)$$

where ρ kg/m^3, cp J/(kg·°K), λ W/(m·°K), μ Pa/s are the density, specific heat capacity at constant pressure, thermal conductivity and viscosity of exhaust gases; λ_{wall} W/m·°K is the thermal conductivity of the block wall; α_{wall} W/(m^2·°K) is the heat transfer coefficient of the channel wall; P Pa is the pressure; T_{inner}, T_{gaz}, T_{wall} °K are the outside air, exhaust gas and partition temperature; V, U, W m/s are the x, y, z speed components, q_v W/m^3 is the density of volumetric heat sources of chemical reactions.

In general, the flow in the catalyst channel is described by the nonstationary Navier-Stokes equation (6, 7) and mass transfer (8).

The Navier-Stokes equation is as follows:

$$\rho\left(\frac{\partial v}{\partial \tau} + v\frac{\partial v}{\partial x} + u\frac{\partial v}{\partial y} + w\frac{\partial v}{\partial z}\right) = \rho g_x - \frac{\partial(p+p_f)}{\partial x} + \frac{\partial}{\partial x}\left(2\mu\frac{\partial v}{\partial x} - \right.$$
$$\left. 23\mu\mathrm{div}V + \partial\partial y\mu\partial v\partial y + \partial u\partial x + \partial\partial z\mu\partial v\partial z + \partial w\partial x \right), \ (6)$$

$$\rho\left(\frac{\partial u}{\partial \tau} + v\frac{\partial u}{\partial x} + u\frac{\partial u}{\partial y} + w\frac{\partial u}{\partial z}\right) = \rho g_y - \frac{\partial(p+p_f)}{\partial y} + \frac{\partial}{\partial y}\left(2\mu\frac{\partial u}{\partial y} - \right.$$
$$\left. 23\mu\mathrm{div}V + \partial\partial x\mu(\partial u\partial x + \partial v\partial y) + \partial\partial z\mu(\partial u\partial z + \partial w\partial y) \right), (7)$$

$$\rho\left(\frac{\partial w}{\partial \tau} + v\frac{\partial w}{\partial x} + u\frac{\partial w}{\partial y} + w\frac{\partial w}{\partial z}\right) = \rho g_z - \frac{\partial(p+p_f)}{\partial z} + \frac{\partial}{\partial z}\left(2\mu\frac{\partial w}{\partial z} - \right.$$
$$\left. 23\mu\mathrm{div}V + \partial\partial x\mu(\partial w\partial x + \partial w\partial z) + \partial\partial y\mu(\partial u\partial y + \partial w\partial z) \right), (8)$$

where ρ, c_p, λ, μ are the density, specific heat at constant pressure, thermal conductivity and viscosity of the exhaust gas; P Pa is the pressure; g_x, g_y, g_z m/s^2 are the components of mass forces; V, U, W m/s are the velocity components.

During flow, the mass conservation equation (mass transfer) is written as the distribution of the concentration of the i-th substance in the exhaust gas stream in the channel for each component:

$$\frac{\partial c_i}{\partial \tau} + v\frac{\partial c_i}{\partial x} + u\frac{\partial c_i}{\partial y} + w\frac{\partial c_i}{\partial z} = D_m\left(\frac{\partial^2 c_i}{\partial x^2} + \frac{\partial^2 c_i}{\partial y^2} + \frac{\partial^2 c_i}{\partial z^2}\right) - r, (9)$$

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

The equation for the distribution of the concentration of the i-th substance on the boundary porous layer is as follows:

$$\frac{\partial c_i}{\partial \tau} + v\frac{\partial c_i}{\partial x} + u\frac{\partial c_i}{\partial y} + w\frac{\partial c_i}{\partial z} = D_m\left(\frac{\partial^2 c_i}{\partial x^2} + \frac{\partial^2 c_i}{\partial y^2} + \frac{\partial^2 c_i}{\partial z^2}\right) - r. (10)$$

The equation for the distribution of the concentration of the i-th substance on the active porous layer is as follows:

$$\frac{\partial c_i}{\partial \tau} = -r. \qquad (11)$$

The system of equations should be transformed in such a way as to establish dependencies between the mathematical model and the design parameters of the exhaust gas post-processing systems, to relate the theoretical parameters, which will allow optimizing the system parameters at the design stage.

The complete model constructed in this way describing the processes in the catalytic unit of the neutralizer seems to be quite complex and requires a large number of

calculation cells and estimated time, even if the grid is uneven.

Difficulties in the three-dimensional study of nonstationary transient modes and effects associated with both channel geometry and fundamental obstacles are significant: computational complexity and memory costs; unstructured mesh generation for areas with complex geometry; three-dimensional calculation of diffusion, the complexity of constructing high-order schemes on unstructured grids; inefficient parallelization of the computational algorithm [30, 32].

Based on these considerations, it is necessary to build a simplified model that allows carrying out a sufficient number of analyses at the design stage with acceptable accuracy, taking into account the accepted initial assumptions.

Consideration of the system of equations, taking into account the previously established assumptions, will greatly simplify the system and allow for taking into account the main features of the designed system.

Let us make additional assumptions;

6. Let us proceed to the axisymmetric two-dimensional problem by excluding the y coordinate (and, accordingly, the triangular channel) from consideration.

7. Let us neglect the transfer of energy in the z direction, taking into account its substantial smallness in comparison with a convective transfer in this direction.

8. Let us present the diffusion equations taking into account the kinetics from the three-layer model to the model of one layer of a heterogeneous reaction, taking into account the correction of the mass flow.

9. The heat transfer equations will also be reduced to one, replacing the heat sink through the block array and the heat of reaction with distributed sources in the stream.

10. The temperature of the unit is equal to the temperature of the exhaust gas.

Then the equations will have the following form:

The energy equation (reduced) for the flow is as follows:

$$\rho c_p \left(\frac{\partial T}{\partial \tau} + v\frac{\partial T}{\partial x} + w\frac{\partial T}{\partial z}\right) = \frac{\partial}{\partial x}\left[\lambda\left(\frac{\partial T}{\partial x}\right)\right] + \frac{\partial}{\partial z}\left[\lambda_{\text{wall}}\left(\frac{\partial T}{\partial z}\right)\right] + q_{\Sigma v} + \alpha_{\text{wall}}\left(T_{\text{wall}} - T_{\text{gas}}\right) + \alpha_{\text{inner}}\left(T_{\text{inner}} - T_{\text{gas}}\right). \quad (12)$$

The Navier-Stokes equation is as follows:

$$\rho\left(\frac{\partial v}{\partial \tau} + v\frac{\partial v}{\partial x} + w\frac{\partial v}{\partial z}\right) = \rho g_x - \frac{\partial(p+p_f)}{\partial x} + \frac{\partial}{\partial x}\left(2\mu\frac{\partial v}{\partial x} - \frac{2}{3}\mu\text{div}V\right) + \frac{\partial}{\partial z}\left[\mu\left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial x}\right)\right], \quad (13)$$

$$\rho\left(\frac{\partial w}{\partial \tau} + v\frac{\partial w}{\partial x} + w\frac{\partial w}{\partial z}\right) = \rho g_z - \frac{\partial(p+p_f)}{\partial z} + \frac{\partial}{\partial z}\left(2\mu\frac{\partial w}{\partial z} - 23\mu\text{div}V + \partial\partial x\mu(\partial w\partial x + \partial w\partial z)\right). \quad (14)$$

The mass equation in the porous layer is as follows:

$$\frac{\partial C_i}{\partial \tau} + v\frac{\partial C_i}{\partial x} + w\frac{\partial C_i}{\partial z} = D_{m\Sigma}\left(\frac{\partial^2 C_i}{\partial x^2} + \frac{\partial^2 C_i}{\partial z^2}\right) - k_i e^{-E_i/RT}\prod\theta_i, \quad (15)$$

where D_m m^2/s is the molecular diffusion coefficient; r $mol/(m^3 \cdot s)$ is the invariant rate of a chemical reaction.
Let us write equations in a dimensionless form suitable for analysis:

$$\frac{1}{Fo}\frac{\partial T}{\partial t} + RePr\left(V\frac{\partial T}{\partial X} + W\frac{\partial T}{\partial Z}\right) = \frac{\partial^2 T}{\partial X^2} + \frac{\partial^2 T}{\partial Z^2} + Q_{\Sigma v} + Nu_{\text{wall}} + Nu_{\text{inner}}, \quad (16)$$

$$St\frac{\partial V}{\partial t} + V\frac{\partial V}{\partial X} + W\frac{\partial V}{\partial Z} = \frac{1}{Re}\left(\frac{\partial^2 V}{\partial X^2} + \frac{\partial^2 W}{\partial Z^2}\right),$$
$$St\frac{\partial W}{\partial t} + V\frac{\partial W}{\partial X} + W\frac{\partial W}{\partial Z} = -Eu\frac{\partial P}{\partial Z} + \frac{1}{Re}\left(\frac{\partial^2 V}{\partial X^2} + \frac{\partial^2 W}{\partial Z^2}\right),$$
$$St\frac{\partial C_i}{\partial t} + V\frac{\partial C_i}{\partial X} + W\frac{\partial C_i}{\partial Z} = -Da + Bo\left(\frac{\partial^2 C_i}{\partial X^2} + \frac{\partial^2 C_i}{\partial Z^2}\right).$$

Here
$St = d/V_d\tau_d$ is the Strouhal number

$Fo = a\tau_d/d^2$ is the Fourier number

$Nu = \alpha_{\text{wall}}D/\lambda$ is the Nusselt criterion (channel)

$Nu = \alpha_{\text{inner}}d/\lambda$ is the Nusselt criterion (block)

$Re = V_d d/\nu$ is the Reynolds number

$Eu = P_{\Sigma}/(\rho V_d^2)$ is the Euler number

$Bo = D_{m\Sigma}/(dV_d)$ is the Bodenstein criterion

$Da = (k_i e^{-E_i/RT}\prod\theta_i d)/(C_0 V_d^2)$ is the Damköhler number

$Q = q_{\Sigma}d^2/(\lambda T_0)$ is the dimensionless stock source

The exhaust gas parameters, depending on the temperature, are determined by the following relationships:

$$\rho = 1 \cdot 10^{-6}T^2 - 0.003T + 2.0218, \quad (20)$$

$$\mu = 3.49 \cdot 10^{-8}T - 6.6539 \cdot 10^{-6}, \quad (21)$$

$$C_p = 0.28T + 966.12, \qquad (22)$$

$$\lambda = 0.00158e^{0.0016T}, \qquad (23)$$

$$Pr = 0.76315e^{-0.00023T}, \qquad (24)$$

$$Sc = 0.90215e^{-0.00023T} \qquad (25)$$

3. RESULT ANALYSIS

Let us determine the speed through the channel of the unit via the flow rate G, engine speed n and engine displacement V_n. The throughput cross-section area of the unit is equal to

$$F_b = \frac{\pi D^2}{4}(1 - 4d_j^{1,5}\delta), \qquad (26)$$

where d_j is the number of cells per square meter; n is the number of revolutions of the engine, min^{-1}; V_n is the engine displacement, m^3.

The value $4d_j^{1,5}\delta$ that is taking into account the thickness of the channel walls ($\delta \sim 10^{-5}$ m) is significantly less than 1, therefore, in the future, with one exception, it will be excluded from reasoning.

Then speed is

$$V_d = \frac{2V_n n}{F_b} = 2Un, \qquad (27)$$

where $U = \frac{V_n}{\frac{\pi D^2}{4}}$ is the coefficient of multiplicity, indicating the ratio of the scales of the volume of the engine and the catalytic unit. In design practice, reducing the coefficient of multiplicity increases the efficiency of the neutralization system. The number U lies in the range of 0.06...1.6.

Note that the size of the square channel cell is

$$d = \frac{1}{\sqrt{d_j}}. \qquad (28)$$

Then the Strouhal number, which determines the scale of the nonstationary term in the model equations and determines the inertia of the processes, will be (Figures 5-7):

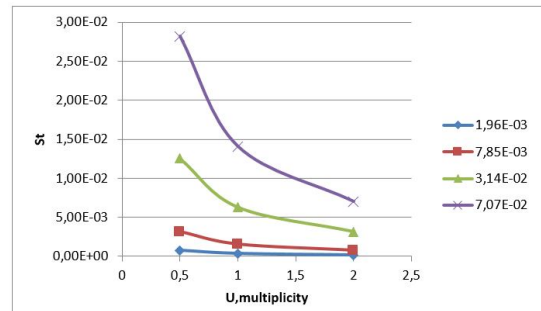$$St = \frac{F_b}{PV_n\sqrt{d_j}}. \qquad (29)$$

Figure 5: St value with an average engine volume and cell density of 450 per inch and a different block area
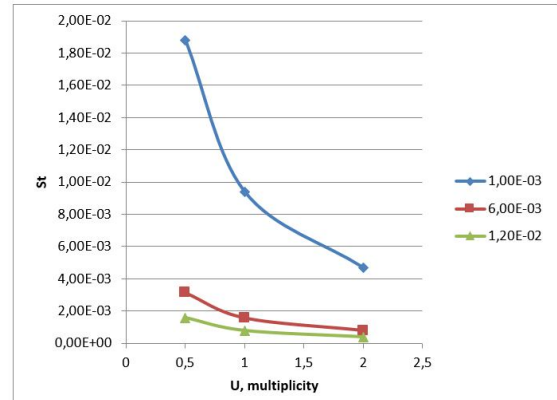

Figure 6: St value with an average block area and cell density of 450 per inch and different engine volumes
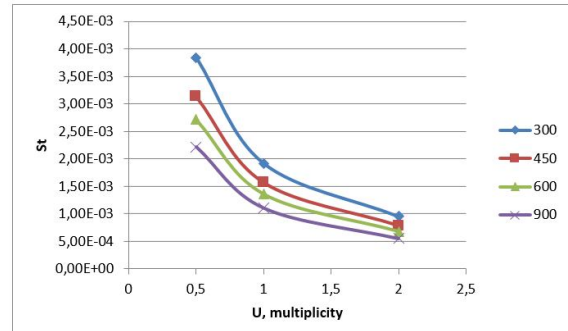

Figure 7: St value with an average block area and engine displacement and different cell densities

The St number does not depend on temperature, so the scale of nonstationarity for the equations of gas dynamics does not change when the temperature level changes, depends only on the geometric parameters of the system. To build a few inertial systems (working well on variable test cycles, such as NEDC), it is necessary to select a set of geometric parameters based on the minimum values of the Strouhal number.

In contrast to the Strouhal number, the Fourier number determines the scale of the nonstationary term in the energy equation and depends on the temperature level and engine operating modes (Figures 8-10):

$$Fo = \frac{ad_j}{2nU}. \quad (30)$$

$$Re = vd\rho/\mu. \quad (31)$$

For the discussed case, $v = \frac{Q}{S} = \frac{nV^2}{60}\frac{4}{\pi D^2}$,
Then

$$Re = \frac{nV_n\rho}{7,5\pi D^2\sqrt{d_j\mu}}. \quad (32)$$

The Reynolds number recorded in this way quite accurately describes the operating mode (flow rate) and the geometric parameters of the catalytic unit, for example, depending on temperature (Figures 11-14).
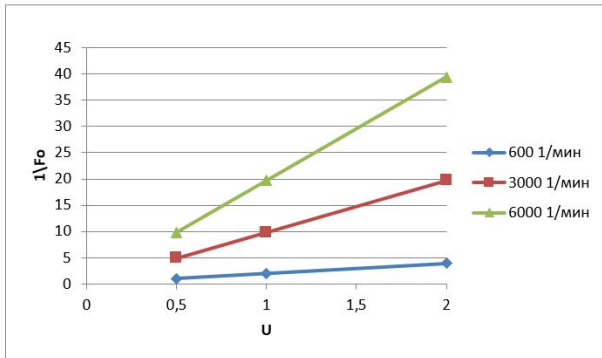

Figure 8:. 1/Fo value depending on revolutions at T = 500 °C and cell density 450 per inch
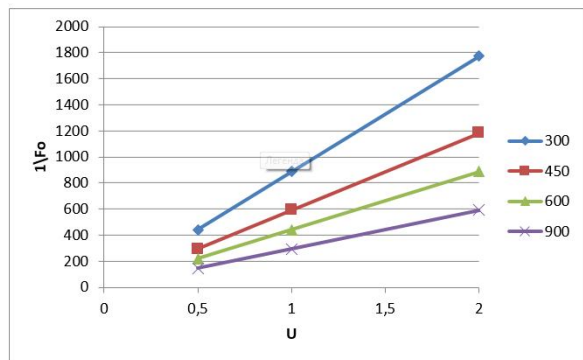
Figure 9: 1/Fo value depending on revolutions at T = 500 °C and cell density 450 per inch

Figure 11: The Re number of the cell density at a constant block area and revolutions at a temperature of 500 °C

Figure 12: The Re number of the diameter of the block at a constant cell density and engine speed

Figure 10: The value 1/Fo depending on temperature at revolutions n = 3,000 1/min and cell density 450 per inch

The influence of the nonstationary term of the energy equation is most significant at low temperatures, low cell density and high exhaust gas consumption (revolutions). The range of change is significant – three orders of magnitude. Changes in temperature fields, especially at the heating stage, in the neutralization system are very mobile.The Reynolds number affects the convective terms of the energy equation, and the second (diffusion) terms of the equation of moments of motion. Let us write the values of the Reynolds number for a single channel of the catalytic unit:
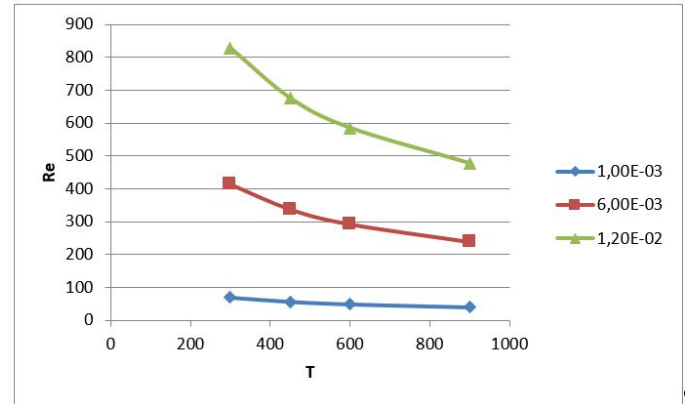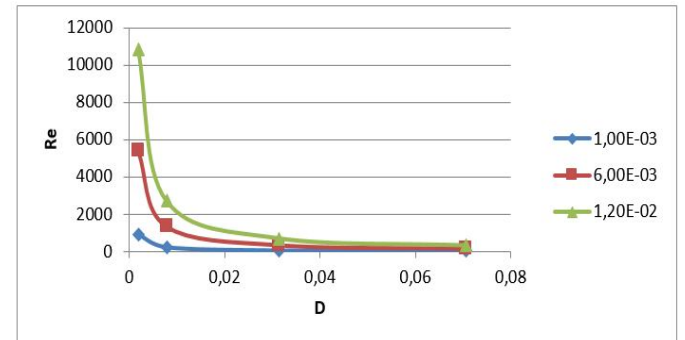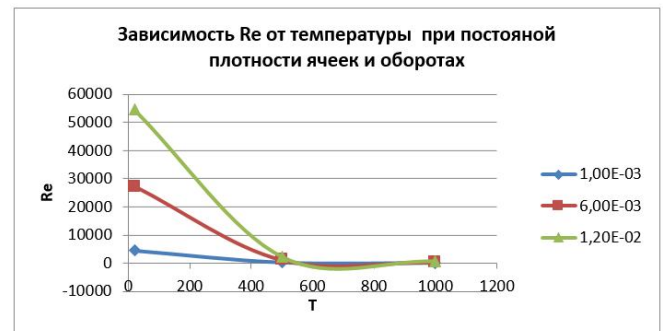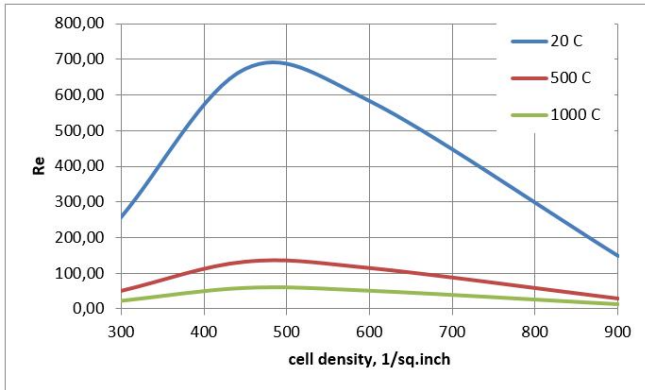

Figure 13: The Re number dependence on the temperature at a constant cell density and speed

Figure 14: Dependence of Re on the density of block cells and different temperatures

The flow parameters determined by the Reynolds number significantly affect heat transfer and gas dynamics and, accordingly, the kinetics of the processes (temperature, pressure). The ratio of limiting factors (diffusion or convection) depends on the Reynolds number. The selection of parameters must be carried out taking into account this factor, reducing the Re number.

The Damköhler number describes the relationship between the rate of change of the mass of a component due to the reaction and due to the mass of the component entering the reactor. For design practice, it is interesting to increase the Da number, for example, by increasing the unit area and the reaction rate due to temperature (Figures 15-16).

The Da number can be written as the following relation:

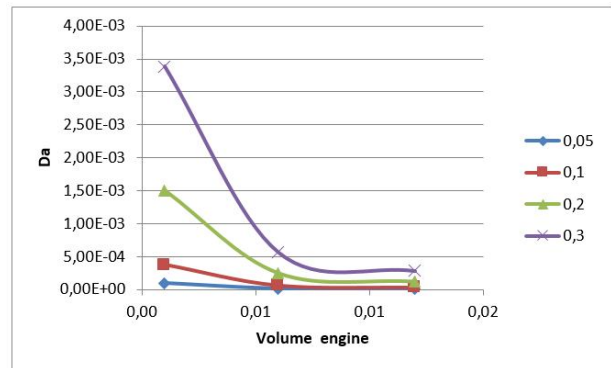$$Da = \frac{rF}{\sqrt{d_j 2nV_{engine}C_0}}. \qquad (33)$$
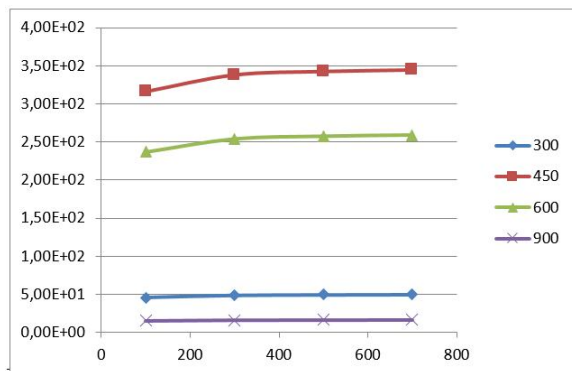
Figure 15: Dependence of the Da number on the cell size and temperature at a speed of 95 m/s
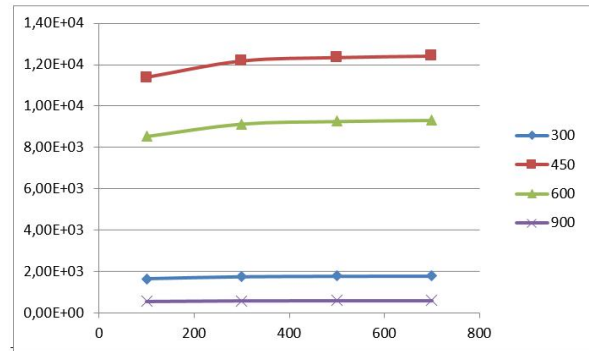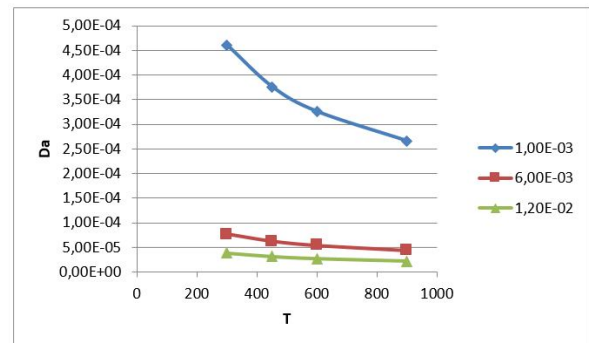

Figure 16: Dependence of the Da number on the cell size and temperature at a speed of 10 m/s

It is of interest to record the Da number, which relates the degree of conversion with the system parameters (Figures 17-20).

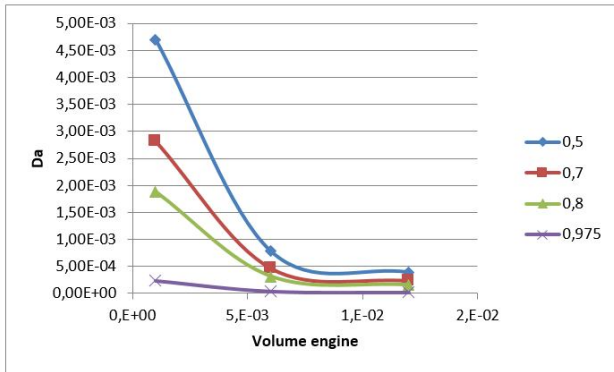$$Da = \frac{\chi F}{V_n P \sqrt{d_j}} \qquad (34)$$

Figure 17: Dependence of the Da number on engine displacement and unit diameter at P = 1 and 450 cells per inch and 95% conversion
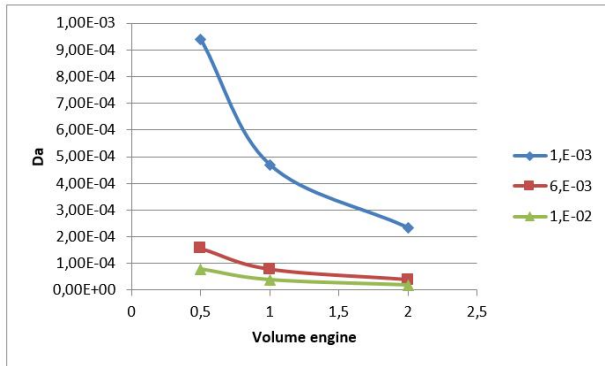

Figure 18: Dependence of the Da number on temperature and cell density at P = 1 and conversion of 95%

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Figure 19: Dependence of the Da number on engine displacement and the degree of conversion

Figure 20: Dependence of the Da number on engine displacement and multiplicity at P = 1 and 95% conversion

The dependence of the number on geometric parameters is quite significant (10 times). The correct ratio of geometry and optimization will help to build a system with optimal parameters.

The Bodenstein criterion describes the relationship between diffusion and convection in a model (Figures 21-23). Diffusion is the mass conductor between the volume transferred to the reaction zone by the exhaust gas flow and the zone of chemical transformations on the catalyst surface. A balance of mass transfer must be maintained for optimal ratios of reaction rate and convection.

$$Bo = \frac{D_m}{V_d d} = \frac{D_m F \sqrt{d_j}}{2nV} \quad (35)$$

The diffusion coefficient for the i-th component is determined by the Fuller – Shetle – Giddens formula depending on the temperature:

$$D_m = D_0 \left(\frac{T}{T_0}\right)^{1.75} \quad (36)$$

The coefficient of effective diffusion is:
$$D_{eff} = \frac{\varepsilon}{\frac{1}{D}+\frac{1}{D_k}}, \quad (37)$$
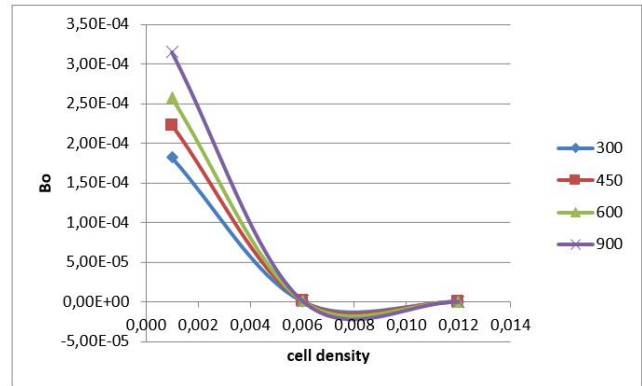
where $\varepsilon = \frac{V_p}{V_{cat}}$ is the coefficient of porosity;

D_k is the diffusion coefficient calculated by the Knudsen formula, taking into account diffusion in narrow pores:

$$D_k = \frac{D_p}{3} \sqrt{\frac{8RT}{\pi M}}, \quad (38)$$

where D_p m is the pore diameter; M mol/kg is the molecular weight of the i-th component.

$$D_k = v/Sc \quad (39)$$

Figure 21: Dependence of the Bo number on the cell density during diffusion of the limiting process
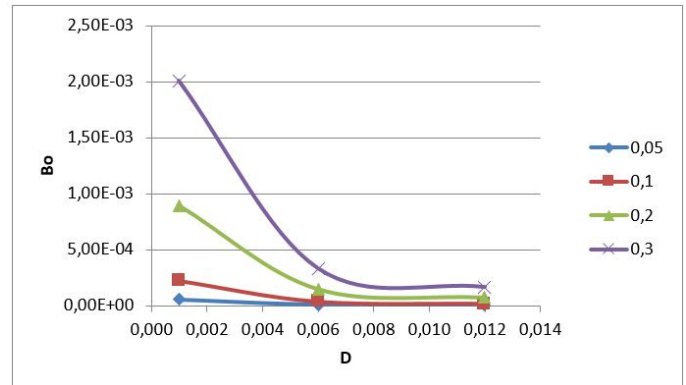
Figure 22: Dependence of the Bo number on the diameter of the block

Figure 23: Dependence of the Bo number on the diameter at different temperatures (diffusion is a limiting factor)

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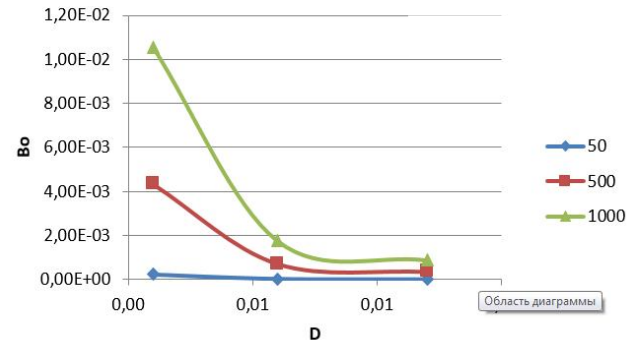The order of the criterion is 2-3 orders of magnitude less than other dimensionless criteria, which reduces its influence, but significantly depends on temperature.

The Nusselt criterion characterizes heat transfer on the inner wall of the channel and on the outer surface of the block:

$$Nu_1 = \frac{\alpha_{inner}}{\lambda\sqrt{d_j}}, \qquad (40)$$

$$Nu_2 = \frac{\alpha_{wall}D}{\lambda}. \qquad (41)$$

When designing, it is practical to use the ratio control

$$\frac{Nu_1}{Nu_2} = \frac{\frac{\alpha_{inner}}{\alpha_{wall}}}{(\sqrt{d_j}\cdot D)}.$$

Design practice shows the need to maintain this ratio significantly higher than 1. The value of the Nu criterion is a function of speed $Nu = f(Re)$.

The smaller is the cell, the faster the block warms up, the larger the block is, the greater the heat loss to the environment is.

4. CONCLUSION

The analysis carried out establishes the main dependencies between the process parameters and the values of geometric parameters of a particular calculation case (engine, revolutions, block and its cell sizes).

These dependencies make it possible at the initial stage to establish priority directions for the design of the catalytic block (block heating rate, efficiency in nonstationary processes). It is possible to preliminarily determine the influence of parameters on the degree of conversion of the designed system.

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