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Calculation of the Operation Parameters of the Catalytic Converters of the Harmful Gas Impurities

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There are theoretically founded principles of catalytic converters designing of harmful gas emissions of various heat devices. Experimental investigations have shown that the smallest aerodynamic losses in the constructions of gas neutralizers are achieved at the using of profiled ceramic blades as working units - carriers of catalysts. To ensure intensive mixing of the flow inside the converter the input edges of the blades grids of the future stages should be located between the output edges of the blades of the grids of the preceding stages.

1. Introduction

Blocks the catalytic purification of gas emissions of any production facilities consist of the following basic parts: – body with inlet and outlet nozzles, inside the working volume of the body in a specific way are work items flowing gases, called catalyst carriers. On the surface of carriers deposited catalytically active layer (layers) of the coating. The task of rational distribution of carriers in the volume of the catalytic converter is to provide maximum degree of conversion of harmful gas emissions while ensuring minimal aerodynamic resistance of the unit itself.
It is necessary the following to create a catalytic converter: to create a production technology of carriers of the given geometry, which providing maximally free passage of gases to selected composition of the catalytically active coating of the carriers provided the maximum degree of conversion of harmful substances contained in the gas. For this purpose it is necessary to formulate and solve the equations describing the process gas flow and heterogeneous transformation of harmful substances taking into account dissipation due to leakage exothermic conversion process.

2. Main part

Gas emissions of heat-energetic objects can contain various active chemical compounds that have a negative influence not only on a human body, but also lead to the destruction the constructional materials. The use of metals in corrosive active environment is not economically feasible because of the need to use special high-alloy, having an appropriate resistance to aggressive agents. Ceramics is relatively affordable and technologically viable material for the creation of structural elements, designed to work in such conditions. By their chemical nature aluminum oxide manifests indifference to the interactions with the aggressive agents in both acidic and basic environments.
Even more inertia to entering into a chemical reaction shows fused α-Al_2O_3, corundum. In addition, this mineral shows the highest resistance to abrasive wear since it has a high strength – to a score of 1 on the Moos scale corundum, inferior in hardness only to diamond.
Writing the equations of heat transfer in the form Eq(1) literally means that in directions transverse coordinate of the second flow space extends to 1 m.

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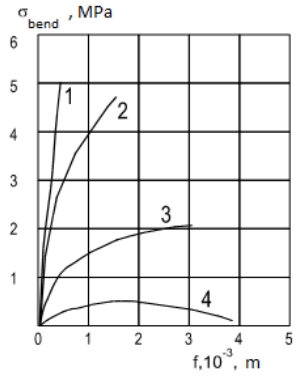

Figure 1: Diagram of deformation in bending corundum ceramics with viscous-plasticity, at temperatures, ºC: 1 – 300; 2 – 500; 3 – 700; 4 – 900

At the present time fundamentally new ceramic materials are produced by means of creating original methods for the synthesis of ceramic elements, especially the production of articles of complicated shapes, carried out at high temperatures and pressures. They are associated with a very broad range of thermo-physical and strengthening characteristics as well have technological, theoretical and technical ones. We have developed a new class of ceramic materials based on α-Al_2O_3, which have certain and controlled level of plasticity of the structure (Figure 1), manifested in different temperature intervals. For a new class of chemically bonded materials the proposed technology of forming ceramic parts of various shapes without the presence of scarce and expensive equipment.

Ceramic materials having a certain degree of high-temperature plasticity is able to relax mobility of pattern applied to them mechanical stresses over the entire temperature interval of their operation. It is founded experimentally proof data in the following: it is proved that the reported to ceramics plasticity of the structure allows the products of any geometrical forms based on it to withstand more than thousand degree gradients of temperature in the range of up to 1,600 ºC, i.e. to demonstrate the abnormally high heat resistance of ceramics.

There are developed technological methods of coating the surface of corundum ceramics with adjustable viscous-plasticity, catalytically active coatings. There are experimentally determined compositions of the catalysts, to ensure substantially complete transformation of polycyclic aromatic hydrocarbons – C3 – C20, chlorinated hydrocarbons and polycyclic aromatic hydrocarbons – i.e., those impurities contained in the exhaust gases of modern waste recycling complexes.

This identified the possibility in principle of operation of catalytic converter gas emissions. The next step is to develop a mathematical model of the process heat in one of the sections of the catalytic converter, perpendicular to the direction of gas motion with account the thermodynamic properties of the converted gas and the availability of heat sources, as well creation of an algorithm of numerical simulation of this process. One of the most common mathematical models in problems of gas dynamics is the continuum approximation, valid for describing gas flows in a wide range of flow settings. Numerical simulation of turbulent flows is carried out by solving the averaged values according to Reynolds– Favre equations of Navier – Stokes augmented by a turbulence model.

However, most turbulence models do not describe with the same degree of adequacy of various types of flows especially flows with intensive flow separation and/or large pressure gradients in temperature. Therefore, there is still need to build new models and computational schemes for the numerical simulation of such flows.

There is created simplified mathematical model of heat dissipation in step of catalytic converter of harmful gas emissions, taking into account thermodynamic properties of gases and the presence of heat sources and an algorithm of numerical simulation of this process.

As a result of the structural analysis of gas-dynamic process taking place in the catalytic stage of the catalyst, decomposition of a complete mathematical model of the process revealed that the main influence on the process has the intensity of heat release in the combustion of carbon (soot) and carbon monoxide contained in the mixture. To describe the process of mixing a two component gas in the present case it is sufficient to use the truncated equations obtained from the Navier–Stokes equations by dropping the viscous and diffuse members – Euler approach with source members.

The design region Ω is a channel with a curved form, located in the Cartesian coordinate system with base in the plane XOZ and the Y-axis which is oriented in the direction opposite to the action of gravity of the Earth.

The computational area is divided into spatial cells and the dimensions of the facets are selected in accordance with a characteristic size of the channel. A complete system of equations describing the unsteady three-dimensional flow of two-component mixture of gases in the Cartesian coordinate system (x, y, z) has the following form:

$$\frac{\partial \vec{a}}{\partial t}+\frac{\partial \vec{b}}{\partial x}+\frac{\partial \vec{c}}{\partial y}+\frac{\partial \vec{d}}{\partial z}=\rho \vec{f} \tag{1}$$

where $\vec{a}$, $\vec{b}$, $\vec{c}$, $\vec{d}$, $\vec{f}$ –vector – columns of the form:

$$\vec{a} = \left[\rho, \rho u, \rho v, \rho w, E\right]^T \tag{2}$$

$$\vec{b} = \left[\rho u, P+\rho u^2, \rho uv, \rho uw, (E+P)u\right]^T \tag{3}$$

$$\vec{c} = \left[\rho v, \rho uv, P+\rho v^2, \rho vw, (E+P)v\right]^T \tag{4}$$

$$\vec{d} = \left[\rho w, \rho uw, \rho vw, P+\rho w^2, (E+P)w\right]^T \tag{5}$$

$$\vec{f} = \left[0, 0-g, 0-gv+e_S/\rho\right]^T \tag{6}$$

t – time; *u*, *v*, *w* – components of velocity vector $\vec{q}$; P, ρ – the pressure and the density; *E* – Is the total energy per unit volume of mixture of gases Eq(7); *e* – internal energy per unit mass of gas; components of a vector $\vec{f}$ – projection of the essence of distributed volumetric sources, g – acceleration of gravity, e_S – intensity of heat release per unit volume of gas due to chemical reaction.

$$E=\rho\left(e+\frac{1}{2}\left(u^2+v^2+w^2\right)\right) \tag{7}$$

The law of transfer of components of the mixture, assuming that the rate of diffusion of the components is much less than the velocity of the mixture has the following form:

$$\frac{\partial(\rho Q)}{\partial t}+\frac{\partial(\rho uQ)}{\partial x}+\frac{\partial(\rho vQ)}{\partial y}+\frac{\partial(\rho wwQ)}{\partial z}=\rho_{Qs} \tag{8}$$

where *Q* – relative mass density of the impurity (the ratio of the density of a gaseous substance impurities to the mixture density), ρ_{Qs} – intensity change of the impurity density due to chemical reaction.

The system of Eqs(1, 8) is unclosed. Add to it the equations that defining thermo-physical property of mixture components. For an ideal polytrophic gas the value e is related to *P* and *ρ* of the mixture by the dependence:

$$e=\frac{P}{(k-1)\rho} \tag{9}$$

Vector Eq(1) is a consequence of the conservation laws of mass, impulse and energy, which can be represented in the integral form for each computational cell:

$$\frac{\partial}{\partial t}\iiint_V \vec{a}dV+\iint_\sigma Bd\vec{\sigma}=\iiint_V \rho\vec{f}dV \tag{10}$$

where *V* – volume of the elementary computational cell; σ – a limiting surface of the cell, which has an outer surface normal $\vec{n}$ $\left(\vec{\sigma}=\sigma\vec{n}\right)$; *B* – tensor of flux density of conservative variables $\vec{a}$, columns of which are vectors $\vec{b}$, $\vec{c}$ and $\vec{d}$, respectively.

The law of transfer of components of the mixture (8) may also be represented in the integral form for each computational cell

$$\frac{\partial}{\partial t}\iiint_V \rho Q dV + \iint_\sigma \rho Q q d\sigma = \iiint_V \rho_{Qs} dV \tag{11}$$

Equations (10, 4) allow the emergence and existence of the discontinuity surfaces of two types: shock waves and tangential discontinuities. Functions satisfying Eqs(10, 11), can be considered as generalized solutions of equations of gas dynamics. The use of integral conservation laws as the starting point for building a differential equations provides a construction of discontinuous solutions without allocation of breaks.

When setting boundary conditions it is believed that the expenditure component of the velocity never exceeds the speed of sound. The boundary conditions at the entrance will ask on the surfaces of the faces adjacent to the boundary of the computational area enters the surrounding air. The incoming flow at the inlet is determined by the values:

– the total enthalpy:

$$I_{00} = \frac{k}{k-1}\cdot\frac{P}{\rho} + \frac{1}{2}\left(u^2 + v^2 + w^2\right) \tag{12}$$

– function of entropy:

$$S_0 = \frac{P}{\rho^k} \tag{13}$$

– the direction of the vector flow velocity – angles α_x, α_z;

– relative mass density of impurity Q ($Q \leq 1$, if there is a gaseous substance impurities, that is carbon monoxide, CO).

The flow parameters at the inlet are determined from Eqs(12, 13) for given α_x,α_z involving ratios for the “left” Riemann invariants. On impervious areas, limiting the calculation area surfaces the conditions of non-flowing: q_n = 0, where $\vec{n}$ – vector normal to this border. The boundary conditions at the outlet are set on the surfaces of the faces adjacent to the boundary of the computational domain, through which it is expected leakage mixture. In the output areas, except atmospheric pressure of Pa, specified or taken from the experiment, ratios were used for the “right” Riemann invariants. As an initial approximation was set in the cells of the computational domain the parameters of the flow inside the occupied volume, corresponding to the inlet conditions in the computational area.

3. The discussion of the results

A complete system of equations of gas dynamics of the interacting mixture of gases was solved numerically by the method of Godunov. Based on the existing developed a software product that implements the described method. It is an integrated, interactive user experience that combines all running modules CAE system (Computer-Aided Engineering) and implements the following functions: generation of source data, modifying data files, viewing data files, running executables as well visualization of data files.

As an illustration of developed methods application and implements of its software product the results of the calculations of the flow in the inter-scapular channels of the catalytic converter of harmful gas emissions from incinerators are considered.

The calculations allowed proposing a form of single element of catalytic converter of the exhaust gases, made in the form of a rectangular parallelepiped with smooth adapters on inlet and outlet for connection to mains supply and removal of gases. The volume of a parallelepiped has been housed ceramic blades (Figure 2).

Figure 2: General view of the ceramic blade - element of the catalysts carrier

The working space of the catalytic converter was filled with four rows of blades. Each row of blades was a grating with parallel end walls. The grating blades have been of two types – convergent (lattices with odd numbers) and diffuser (grid with even numbers). The consecutive alternation of two types of gratings has been

provided near-zero angles of attack at the entrance to each of the grids and, as a consequence, low flow loss of kinetic energy while passing the working fluid through the working space of the converter.
The blade grills have been placed in such a way that the input edges of the blades grids with even numbers were located between the output edges of the blades grids with odd numbers, which provides intensive mixing of the flow in the inter-scapular channels of the grating. A schematic representation of the working space filling of catalytic converter rows of blades are represented in Figure 3.

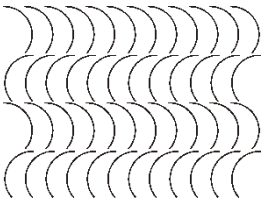

Figure 3: Schematic representation of the working space filling of catalytic converter rows of blades

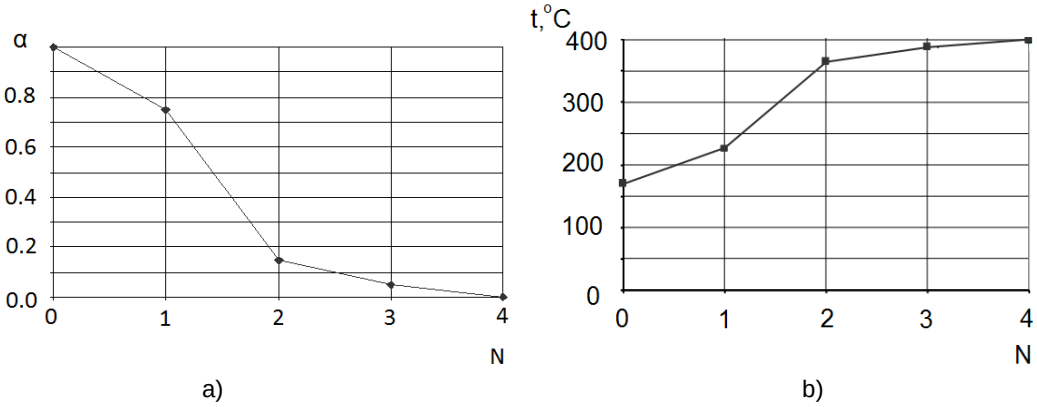

Figure 4: Change of flow parameters on the four steps of the tract of catalytic converter (α is the conversion rate, N is the number of neutralization stages)

There are shown the dependences of relative change of mass density of carbon monoxide in the air stream (a), flow parameters at the inlet and the temperature of the mixture (b) along the route four-stage converter in Figure 4. It is obvious that the bulk of the impurity is burnt in the second stage of converter and for complete combustion of the impurities it is enough four steps.
The calculated basic design parameters and data about the grid profiles:
– chord (*B*) 0.05 m;
– relative pitch ($t^{\circ}=T/B$) 0.2;
– elongation of the blades ($H^{\circ}1=H1/B$) 3.8;
– the bending angle of the middle line of the profile (Θ) is 24°.

Figure 5: The field of static temperature in inter-scapular channel in the middle height of the blade cross-section converging grating profiles

The experimental and calculated investigations were executed for regime of corresponding to angle of fighting at the entrance to first cell $i_1 = 0$ at the $T_1 = 170$ ºC and $M_1 = 0.012$ kg/kmol. There are brought the calculations

results of statistic temperature field of static temperature in the inter-blade channel on average the height of the blade section of the first converging grating profiles on the Figure 5. There was a proportional increase in the temperature downstream due to the exothermic process of neutralization of harmful gases contained in the stream. Calculated absolute temperature increment in a single lattice is $\Delta T = 54$ °C, the experimental value is $\Delta T = 57.5$ °C.

4. Conclusions

There are carried out verification of developed mathematical model and algorithm of numerical solution of heat and mass transfer in the inter-blade channels of the catalytic converter of harmful gas emissions of incinerators. There has been obtained satisfied correspondence of results the numerical and experimental studies.

Analysis of Navier-Stokes equations, methods for constructing of their solutions and their areas of application leads to the conclusion that significant reductions in computation and stored for these purposes the information on the computer should be used for simulation of heat release in catalytic converters Euler equations with source terms. The developed mathematical model, method and algorithm of the numerical solution of heat dissipation in the inter-scapular channels of the catalytic converters. There are obtained the results of computational research.

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