MATHEMATICAL SIMULATION AND THERMAL STATE ANALYSIS OF COMBUSTION CHAMBERS FOR POWER SYSTEMS (ON THE BASIS OF THE NEURAL-NETWORK COMPUTING ARCHITECTURE)

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Abstract. Some problems of thermodynamic, hydraulic and thermal calculations of the thermal state analysis and performance of the liquid-propellant rocket engine design using neural network modeling are detected. The algorithm of the numerical decision of the hydrodynamics equations with representation of the decision on method of weighted residuals on the base of general neuronet's approximation in the whole flow area is developed. There are presented some applications of neural-network algorithms using in thermal calculations of the LRE chamber such as the simulation of hydraulic non-uniformity of fuel distribution among the sprayers of LRE mixing devices.

The presented results were obtained in the frame of the “Creation of a production of the new generation main oil pump using the methods of multi-criteria optimization and unique experimental base” project conducted by "Turbopump" OJSC (Russian Federation Government Resolution №218 from 9.04.2010). Applied scientific research (ASR) is conducted by Voronezh State Technical University in accordance with the contract number 1450 / 300-13 dated 24 February between "Turbopump" and Voronezh State Technical University.

Key words: liquid rocket engine, LRE, neural network modeling, thermal state analysis

The liquid-propellant rocket engine (LRE) chamber is one of the most heat-stressed constructions of combustion chambers for power systems. It is possible to note the following features and specific conditions of heat exchange in the LRE chamber, complicating the use of traditional thermotechnical methods, namely: 1) high velocity of gas stream motion (the speed of combustion products at the nozzle exit of the LOX-LH rocket engine reaches ~4600 m/s); 2) a sharp temperature gradient (from ~1000 K on the wall to ~3600 K in the flow core), and, hence, the presence of thermophysical properties across the boundary layer; 3) the shaped nozzle, significantly different from a cylindrical tube of canonical geometry, for which, as a rule, heat exchange ratios are obtained; 4) the presence of chemically reactive products of combustion in the chamber firebox, i.e. the reactions of dissociation and recombination, accompanied by the absorption or release of heat, which are necessary to be considered. The urgency of the conducted research can be proved by the following facts. Firstly, the complexity of the operating processes in the LRE often makes it impossible to obtain the reliable mathematical models on the basis of classical definitions of mathematics. Mathematical simulation is mainly represented by checking engineering methods of calculation, based on a great number of assumptions, simplifications and empirical relationships, which, in certain cases, do not allow us to reveal the parametrical and functional problems of the complex technical system at the stage of its design. These problems can refer

to: 1) the processes of hydrodynamics and heat exchange in channels, pipelines, a line of gas supply, a cooling path, etc.; 2) the processes of combustion and chemical reaction kinetics; 3) the complex heat exchange between the dissociated combustion products and the combustion chamber wall; 4) the dynamic processes, including those occurring in the most critical modes of actuation, stoppage, speedup and throttling; 5) quickly varying processes, i.e. vibrating and pulsating operational characteristics; etc. Secondly, the Russian engine construction plants make little use of vast experience, gained by these enterprises in designing LRE (for example, Voronezh Construction Department of Chemical Automatics Design Bureau(CADB) has developed more than 60 models of LRE, 30 of which have been brought to mass production). At the same time, this experimental knowledge is widely used by our foreign partners. For instance, the European Space Agency, while developing the LOX-LH LRE «Vulkan» for its «Arian 5» booster, extensively employed the simulation mathematical model of the LOX-LH LRE of the «Energy» launcher. This model has been developed in cooperation with specialists of the CDCA, on the basis of vast experimental data, obtained from the checkup of the «Energy» engine, which gave the opportunity of minimizing the number of development firing tests of the LRE «Vulkan». Currently, the expenditure on the experimental research, conducted at all design phases, accounts for up to 80% of the total cost of LRE development. The production of new LRE costs hundreds of millions of dollars, and the cost of one firing test in Russian conditions is estimated at several millions of roubles. Today, the development of LRE may require tens or hundreds of firing tests and experimental engine models. If we consider the great number of independent experimental works, carried out during the design and operational development of LRE components and assemblies, and also the fact that the experimental results are generally the only source of objective data for the analysis of operational process and working out engineering solutions, the possibility of reducing the number of experimental development works primarily depends and is largely hampered by the lack of reliable parametrical and functional mathematical models of operational processes in the LRE.

The most serious problem of thermophysical process study, closely related to the systematic approach, is the multidisciplinary character of the tasks being analysed, which require complex solution using knowledge from various scientific disciplines: hydrodynamics, heat transmission, chemical thermodynamics, strength study and materials science. The strategy of design optimization may involve the generation of effective methods of numerical calculation for simulating the conjugate heat-and-mass transfer in turbulent flows, as well as calculation of thermodynamic and thermophysical parameter distribution of combustion products, the estimation of convective and radiant heat exchange parameters, and the impact of operating temperature conditions of systems on their deformation mode.

Proceeding from our analysis of the problems, related to integration of mathematical modeling of thermophysical processes into LRE design, the fields of effective neural networks application have been specified, namely:

1. Approximation.

The method of approximation is used wherever experimental data (including reference data) are applied, especially if these are dependencies between variables, or in cases, when the use of nomograms in design calculation is still convenient.

2. Experimental factor models

The fields of application: processing the results of the planned experiment, possible application of non-classical experimental plans, and adaptation for solving the tasks of optimization with the use of neural-network factor models.

3. Mathematical simulation

It is used, firstly, to identify the classical models, which require the complex calculated and experimental data for creating the neural network; and, secondly, in cases when the application of classical mathematical models needs a considerable amount of time, as well as many test runs during the computational experiment or optimization research.

4. The application of neural-network test solutions in methods of weighted residuals for solving the thermophysical equations.

5. The development of neural-network simulation models of functioning to generate the initial data for modeling thermophysical processes in transient modes, as well as for automated test analysis, monitoring and emergency protection of technical systems.

Classical numerical algorithms. The distribution of hydrodynamic parameters in ring headers of mixing and cooling systems of the LRE chamber, as well as in the inter-sprayer zone of the mixer head, is found by solving Navier-Stokes equations of continuity and momentum, for which the marker-and-cell method is used. The detailed numerical algorithm is presented in [1], which also describes the methods of discretization, the formulation of boundary conditions, the stability condition, the coefficient matrix structures of discretized equation sets, the ways of their solution, and other aspects of computation. It is possible to note such sources of errors in the numerical results as discretization errors, numerical diffusion, low accuracy of calculation for singularities and boundaries, the application of mean arithmetical (but not mean integral) values of function products and so on.

The thermodynamical calculation of combustion is performed on the basis of well-known procedure, under the assumption of the equilibrium process and the absence of combustion product ionization. The system of calculation includes the following equations: 1) the equation of dissociation; 2) the equation of matter conservation; 3) the Dalton's Law equation; 4) the equation of total enthalpy conservation. Since the thermophysical calculation assumes the constant mixing ratio within the wall layer, it appears to be another source of errors in numerical results.

According to the theory of V.M. Ievlev, the mathematical model of convective heat transfer is based on the use of the «exact» formula, and the analytical solution of integral equations of the turbulent boundary layer of combustion products. It is quite promising to solve the original differential equation set for the boundary layer of high-speed flow of chemically reactive combustion products in the chamber and the nozzle of the LRE.

Assuming that the wall temperature Tw is much lower than the one of combustion products T_K, the radiant heat flow in the combustion chamber can be found by:

$$q_л = \varepsilon_{ст.эф} \cdot \varepsilon_Г \cdot C_0 \cdot \left(\frac{T_K}{100} \right)^4 . \qquad (1)$$

In this case, $\varepsilon_{ст.эф} = \frac{\varepsilon_{ст} + 1}{2}$ is the effective wall emissivity; $\varepsilon_{ст}$ is the wall emissivity (depending on the material of the wall and the condition of its surface).

Assuming that CO_2 and H_2O are only matters considered in process of radiation, the degree of combustion product emissivity is found by:

$$\varepsilon_Г = \varepsilon_{CO_2} + \varepsilon_{H_2O} - \varepsilon_{H_2O}\varepsilon_{CO_2}$$

where $\varepsilon_{CO_2} = \varepsilon(\rho l, T)$ and $\varepsilon_{H_2O} = \varepsilon(\rho l, T, \rho)$ are empirical dependences, represented as nomograms, which can be used as reference data. In this case, the application of

neurocomputing structure also allows us to obtain the convenient computer databases on the degrees of emissivity for combustion products of different composition.

The analysis of applicable mathematical models and calculation algorithms leads to the obvious conclusion about the possibility of increasing the accuracy and adequacy of mathematical simulation. Primarily, it is necessary to consider the dependence between the irregular distribution of components over mixing head sprayers and jacket cooling paths on non-uniform distribution of thermodynamical and thermal parameters in the fire box, the cooling path and chamber walls. Secondly, it is obvious, that the accuracy of calculated results can be significantly enhanced by removing the sources of numerical errors, mainly connected with discretization of derivatives in solvable differential equations, and, besides, with low accuracy of boundary representation. Another way of increasing the calculation accuracy is the application of high-precision methods of multivariate approximation, based on the neural-network computing architecture.

Neural-network method of weighted residuals (NMWR). In each specific case, the use of NMWR requires the preliminary systematic study, aimed at: 1) defining the number of calculation nodes (i.e. the size of the calculation grid), 2) finding the number of neurals in the network, necessary for attaining proper approximating power, 3) the choice of initial approximations for training neural-network test solution; 4) the selection of the additional criteria in the goal function for regularization of the training procedure, as to avoid possible non-uniformity of the solution; 5) the analysis of possibilities of applying the multi-criteria algorithms of optimization in search of neural-network solution parameters (provided that several criteria of optimization are available). The systematic study, aimed at detecting the computational properties of the NMWR can be schematically represented in fig.1.

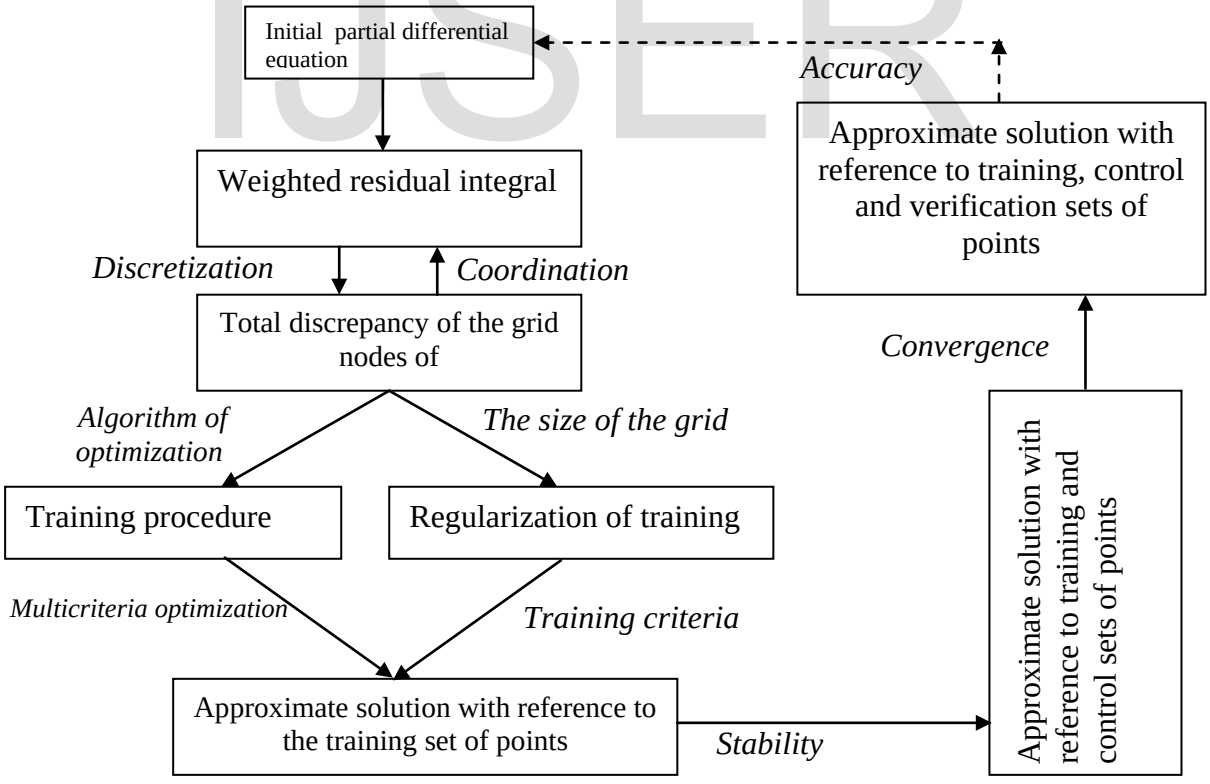

Fig. 1. Methodical points of NMWR application

The application of neural-network algorithms in thermal calculations of the LRE chamber. The simulation of hydraulic non-uniformity of fuel distribution among the sprayers

of mixing devices, along with prognostication of its level, are urgent tasks, related to the design of heat exchangers and fuel distribution systems of combustion chambers in power systems. While solving the problems of LRE efficiency and reliability, caused by imperfection of the carburetion system, it is advisable to conduct the planned experiment, using neural-network response surfaces. The acquisition of the neural-network dependence of discharge, occurring through the separate sprayer of the mixing head, determines the possibility of optimizing the hydraulic sprayer parameters, in order to reduce non-uniformity. The practical outcome of such optimization is the classification of sprayers. The use of sprayer classification solves the problem of non-uniformity of combustion product temperature in the nominal, throttling and forced draft modes. The elaborated procedure of tuning the groups of sprayers, combined into classes, to a specific discharge rate, is used as a supplementary method of mathematical simulation during the final development of the mixer head. It also allows us to reduce non-uniformity of combustion products in the chamber cross-section to the preset level, without reprofiling the air-gas channel of supply collectors, and reconfiguring the sprayer head, which will help to automate the development procedure, while reducing the product cost.

According to the results of experimental spills, which were carried out by the Construction Department of Chemical Automatics for testing the mixer heads of combustion chambers and the gas generator, the research was conducted to examine the impact of the following factors on non-uniformity of discharge distribution over the sprayers, namely: 1) the geometric coordinates of sprayers; 2) the error of hydraulic sprayer parameters, resulting from technological defects; 3) the total mass rate of discharge through the mixer head, 4) the orientation of sprayers in the flow; 5) the reciprocal impact of discharge flows, occurring through different sprayers; 6) the impact of gas blowing of feed lines during the startup; 7) the height of the pre-sprayer cavity; 8) the non-uniformity of static pressure distribution in the pre-sprayer cavity and the feed line. The statistical analysis testifies to considerable redistribution of discharge through the sprayers of the mixer head, in comparison with the autonomous spill of sprayers. Meanwhile, in different modes of spill, the pattern of redistribution does not practically vary. For example, the peripheral sprayers demonstrate the reduced rate of component discharge, while in central ones, the rate of discharge is higher, respectively. During experimental testing, the measurements of differential pressure in sprayers were conducted. The analysis of resulting dependencies shows that the pressure in the mixer head changes insignificantly, and, at least, the redistribution of the component over the sprayers can not be only reduced to non-uniformity of pressure distribution. Obviously, the overspeed of the sprayer flow leads to reduction of their discharge rate, and vice versa. The indicated effect is well-known, however, there are no numerical dependencies of discharge rate on the sprayer flow velocity, as specified for coordinated work of sprayers in the mixer head. The available mathematical model, derived from momentum equations and experimental results of discharge distribution over the sprayers, allows us to obtain the neural-network dependence $\overline{EPS} = f(W)$, in which $\overline{EPS} = \frac{EPS_i}{EPS_{iAAB}} = \frac{\overline{Q}_i}{\overline{Q}_{iAAB}}$ is the coefficient of relative permeability of the sprayer, and W is the velocity of sprayer flow. After its detection, in order to simulate the discharge distribution over the sprayers, it is sufficient to use the equation of mass conservation, with regard to outflow through the sprayers. Thus, the use of the neural-network approximating dependence between the sprayer discharge rate and the speed of its flow makes it possible to considerably facilitate the procedure of measuring the discharge, occurring through the peripheral sprayers. The figure 2 presents the results of using the NMWR for estimating the velocity field in the inter-sprayer space of the 19-sprayer mixer head.

To calculate the component distribution k_m and the intensity of discharge, occurring through the cross-section of the combustion chamber, $\dot{g}$, the general regression neural network (GRNN) is applied. Recently, binary fuel sprayers have been used in the majority of the LRE, thus, it is possible to specify the central coordinate positions of sprayers, located in the injector bottom (r_i, θ_i), as k_{mi} and $\dot{g}_i = \dfrac{\dot{m}_{i\Sigma} \cdot n}{F_{KC}}$, where $\dot{m}_{i\Sigma}$ is the total discharge through the sprayer *i*, and *n* is the number of binary fuel sprayers in the mixer head (provided the sprayers are located in the concentric circles, and the spacings between them are nearly equal). Further, the GRNN is trained, i.e. Gaussian nuclear function is placed at each point, where a sprayer is located. It is assumed, that the values k_{mi} and $\dot{g}_i$, specified for the sprayer *i*-, testify to some confidence in the fact, that the response surfaces, $k_m(r, \theta)$ and $\dot{g}(r, \theta)$, have a certain height at the point given; and this confidence abates when moving aside the central point location.

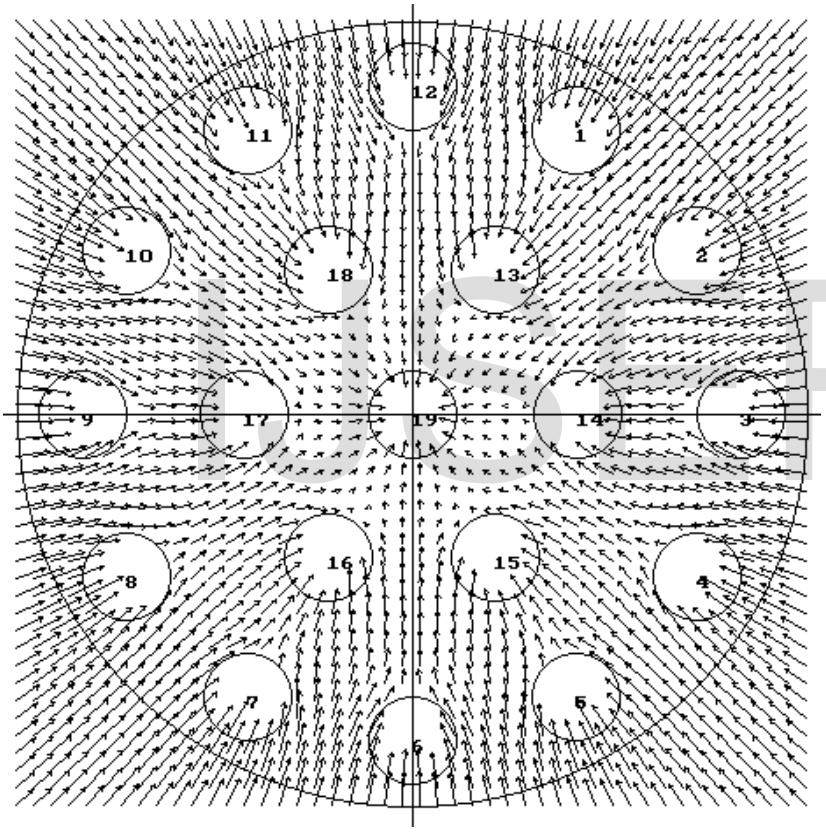

Fig. 2. The calculated velocity distribution in the inter-sprayer space

The GRNN copies all the results of training observations within itself, and employs them for evaluating the response at the arbitrary point of the combustion chamber cross-section. The output of the network is obtained from

$$y = \frac{\sum_{s=1}^{K} y^s \varphi\left(\left\|\mathbf{X} - \mathbf{X}^s\right\| / \sigma\right)}{\sum_{s=1}^{K} \varphi\left(\left\|\mathbf{X} - \mathbf{X}^s\right\| / \sigma\right)}. \qquad (2)$$

where ($\left(\mathbf{X}^s, y\right)$ are the points of the training sample. The only control parameter of training is the deflection magnitude of the Gaussian function σ (the parameter of function smoothing). It is selected as equal to 3 spacings between the sprayers. As can be seen, this approach,

involving the use of the GRNN, incorporates all the concepts of theory, worked out by V.M. Ievlev for calculating the distribution of k_m and $\dot{g}$ in the cross-section of the combustion chamber.

The neural-network computational structures can be applied for obtaining the calculation algorithms in the conditions of non-uniform distribution of components, the discharge intensity in the chamber cross-section, and the irregular discharge distribution over the channels of the cooling path. In this case, it is possible to use the first ($q_K = B\frac{\varphi_1}{\left[\int_0^{\bar{x}} \varphi_3 d\bar{x}\right]^{0,15}} \frac{P_K^{0,85}}{\overline{D}^{1,82} d_{кр}^{0,15}} \frac{S}{\Pr^{0,58}}$) and the second ($q_K = B\frac{\left(1-\beta^2\right)P_K^{0,85}}{\overline{D}^{1,82} d_{кр}^{0,15}} \frac{S}{\Pr^{0,58}}$) approximation formulas by V.M. Ievlev. These formulas demonstrate the impact of non-uniformity on the thermophysical parameters of combustion products. $S = 2{,}06538\frac{\left(I_{0\Gamma} - I_{CT}\right)\mu_{0\Gamma}^{0,15}}{\left(R_{0\Gamma}T_{0\Gamma}\right)^{0,425}\left(1+\overline{T}_{CT}\right)^{0,595}\left(3+\overline{T}_{CT}\right)^{0,15}}$.

The coefficient of heat transfer to a liquid is defined by the Nusselt-Craussold formula,

$$\alpha_{ж} = 0{,}023(\rho w)^{0,8}\frac{\left(c_p^{0,4}\lambda^{0,6}\right)}{\mu^{0,4} d_{\Gamma}^{0,2}}$$

and it is also a variable value in the azimuthal direction, since the rates of discharge, occurring through the cooling channels, are different due to hydraulic non-uniformity. If we use the principles of quasi-two-dimensional formulation of heat transfer problem, then, for each design section of the chamber, it is possible to perform the calculation of convective thermal flow toward the chamber wall, with regard to parameters of the wall layer. The wall layer is determined by its adjacent sprayer (provided that binary fuel sprayers are used, being located in the concentric circles). The parameters of heat transfer to a liquid are determined with account of local (but not average) rate of discharge in the cooling channel. Next, the «stitching» of the obtained solutions, specified for temperatures of chamber walls, is performed, and the resulting thermal field of the construction is applied to calculate the parameters of heat-stressed state. Specific computational algorithms are based on iterative calculations, which require the analytical approximating dependencies of the empirical reference data. If thermophysical properties depend on a single parameter (let us say, on temperature), then the calculation of approximations, made by means of the least-squares method, does not cause any problem. For approximation of non-unidimensional dependencies, it is effective to apply the neural-network computational structure. For example, as part of our work, the neural-network formulas $S_{NET}(T_{cm}, \alpha)$ and $K_{NET}(p,T)$ have been obtained for some rocket propellants and coolants. During our research, the neural-network databases have been created for emissivity degrees, $\varepsilon_{CO_2} = \varepsilon(\rho l, T)$ and $\varepsilon_{H_2O} = \varepsilon(\rho l, T, \rho)$, as well as for $\beta_{\rho H_2O}(\rho_{H_2O}, \rho_{H_2O} \cdot l, T)$, the coefficient, which regards the increase of water steam emissivity due to broadening of emission bands, occurring with the rise in temperature or pressure. These databases can be conveniently used instead of well-known nomograms or tables.

To make a more complete account of multidisciplinary aspects of the operational process of the LRE chamber, it is possible to use the theory, consisting of four coherent clusters, as to increase the validity of thermal state analysis of the combustion chamber. The «hydrodynamic» cluster stems from Navier-Stokes equations, with the use of an algebraic exponential model of turbulence, as well as a κ-ε model. The simulation of hydrodynamic characteristics of collectors is based on equations of variable-mass flow. As a result of calculation, the following characteristics are defined: 1) the irregular coolant distribution over the channels of the cooling jacket; 2) the non-uniform distribution of discharge over the

sprayers of the mixer head. The results, obtained as part of the «hydrodynamic» cluster, are initial for all other clusters. The next, «thermal and gas dynamics» cluster is based on the standard LRPE procedure, which involves the thermodynamic calculations for the combustion chamber, the nozzle exit and the critical section; it also includes the definition of the cross-section parameters by the chamber length, on the basis of familiar gas-dynamic functions. This cluster uses the results of calculations on non-uniformity of discharge distribution over the sprayers, obtained as part of «hydrodynamic» cluster, in order to determine the non-uniformity of discharge intensity distribution, the ratio of components, and, consequently, the temperature of combustion products over the chamber cross section. The results, relevant to «thermal and gas dynamics» cluster are the input data for another cluster, associated with heat exchange. The cluster «heat exchange» is based on the convective heat exchange theory by V.M.Ievlev, and the radiant heat exchange theory by L.F.Frolov. The results of calculations are temperature values of the external and internal chamber walls. The cluster «heat exchange» applies the data of such clusters as «hydrodynamics» (i.e. the irregularity of flow over the channels of the cooling jacket), «thermal and gas dynamics» (i.e. the irregularity of thermophysical properties of combustion products over the chamber cross-section), and «strength» (i.e. the transformation of cooling path geometry). The results, obtained as part of the «heat exchange» cluster are the input data for another cluster, i.e. «strength». Both of these clusters are critical, due to possibility of monitoring the overheating of the chamber walls. The range of problems, included in the «strength» cluster with regard to iterative specification of results, relevant to «heat exchange» cluster, and the variation of heat-stressed state parameters over the rated cross-section. The calculation of local deflections involves the neural-network transfer function, showing the dependence of the wall temperature on the variation of the flow section of the cooling channel. The algorithm of the «strength» cluster includes the results of all remaining clusters, and it completes the procedure. At this stage, the most critical elements and possible defects of the structure are detected.

The integration of thermodynamic, hydraulic, thermal and strength calculations into one computational system allows us to carry out the complex analysis of the thermal state and performance of the LRE, aimed at enhancing the reliability of functioning and rational selection of design parameters in the conditions of high intensity of the operational process.

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