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INNOVATIVE SYSTEM OF COMPUTER MODELLING OF MULTIPHYSICS PROCESSES FOR CONTROLLED ELECTROCURRENT TREATMENT OF MELTS

Introduction. *The widespread use of cast products made of aluminum and its alloys requires ensuring a high-quality structure of the castings, on which their operational properties depend. Controlling the process of forming a high-quality structure of castings is possible, in particular, by the method of electrocurrent treatment of melts.*

Problem Statement. *The melt medium being inaccessible for direct measurement of the processing parameters, the only way to realize the control of treatment conditions is numerical simulation of these parameters. However, the complexity and interdependence of multiphysics processes of melt electrocurrent treatment have led to an unconventional approach to the formulation of their mathematical models and computational procedures. These circumstances have determined the features of the tasks for the construction of appropriate computer models and their application.*

Purpose. *The development of a new pattern-modular system for computer modeling of multiphysics processes of electric current treatment of melts to control the conditions of the formation of a qualitative structure of castings.*

Materials and Methods. *The material of the research is a set of model problems of multiphysical processes of electrocurrent treatment and their ontology, the integral equations and their properties, as well as databases on the parameters of simulated objects, which describe these processes. The method of ontological taxonomy has been used to create a taxonomic codifier, with the help of which model problems and mathematical tools for their solution have been systematized. Based on the signs of similarity, the method of formalization of integral equations of coupled multiphysics processes has been applied.*

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Results. *The unified patterns of basic algorithmic procedures and a library of program modules for computing operations of partial tasks, for which a unique code is assigned according to the codifier have been developed. Combining the patterns with different modules that are identified by the indicated codes has made it possible to form a wide range of computer models reflecting multiphysics processes. A flexible system for computer modeling of multiphysical processes has been built and its efficiency for simulating the modes of electrocurrent treatment of melts has been confirmed.*

Conclusions. *The results obtained have enabled controlling the conditions of electrocurrent treatment of melts to form a high-quality structure of cast metal.*

Keywords: electrocurrent treatment, melt, multiphysical processes, taxonomic codifier, mathematical models, computer modeling, pattern, module.

In various fields of production and economic activities, cast products of aluminum and its alloys have been widely used. In this regard, the problem of obtaining a high-quality structure of castings, on which their operational properties depend, is a problem to be urgently solved [1, 2]. The studies of recent years have proved that it is possible to control the process of forming the casting structure by external physical influences on the metal in a liquid state, since there is a phenomenon of inheritance of the physical features of the melt in the casting properties [1—4]. In this regard, the energy treatment of melts by means of electromagnetic fields is of great interest.

From various options of electromagnetic influences, electric current treatment (ECT) of metal melt has been identified as a particularly promising method for obtaining a qualitative structure at the stage of crystal formation [3, 5]. It has been established experimentally that the distribution of current and electrodynamic forces caused by it in the course of melt treatment significantly affects the formation of the casting structure during its further hardening [5, 6]. The ECT means electric current passing directly through the melt by means of electrodes immersed in it. There may be used the current of different types (direct, alternating, pulsed). So, by choosing the electrode system and the type of current, it is possible to control the distribution and parameters of the primary (electric) field and, accordingly, the thermodynamic state of the melt, thereby purposefully influencing the course of crystallization processes to form the specified or desired characteristics of the cast metal structure [5, 7]. Thus, there are prerequisites for controlling the processes of the casting structure formation by regulating the parameters of the ECT conditions.

The specified method of treatment is a complex process of several physical fields interaction in a liquid metal medium, which covers poorly studied aspects of the electromagnetic fields cross impact in a medium with changing parameters. When current passes in the melt, interrelated physical phenomena occur in it: the appearance of self-inductive EMF and magneto-hydrodynamic flows that cause mixing of the layers and redistribution of temperatures, changes in conductivity and viscosity of the medium. In addition, heterogeneous macro- and micro-inclusions and autogenic formations are inevitably present in the liquid melt matrix [5—7] migrate through the volume and cause local anomalies in the medium parameters.

The described ECT process is essentially multiphysical, i.e. such that is realized by the simultaneous joint action of conjugate physical fields of different nature [8, 9]. The controlling of such a process is a complex scientific and technical task that has an interdisciplinary nature and requires *a thorough understanding of the internal content* of physical phenomena and processes occurring in the melt during its treatment. At the same time, experimental determination of the consequences and results of certain physical influences encounters fundamental difficulties, because they can be obtained only *a posteriori,* by analyzing the structural properties of the finished castings, since the internal volume of high-temperature melt for direct measurement of local pa-

rameters of interacting media before its solidification is *physically inaccessible*.

Therefore, the selection of the optimal ECT mode can be carried out only manually, when manufacturing particular parts or small batches of casting products. On the other hand, the introduction of such a method in the technologies of mass production of castings is extremely difficult due to the large number of factors affecting these processes and parameters that need to be monitored and regulated [1, 7]. Under such conditions, the *only available means* of revealing the effect of control actions on the controlled parameters and the final results of the ECT is the use of computational methods. Moreover, the multifactorial nature of ECT processes ***necessitates*** the creation of an automated system for computer simulation and control the modes of melt treatment, which, of course, should be based on adequate mathematical models of physical fields that actually perform control functions.

These circumstances clearly define a problematic situation, the solution of which can only be achieved in ***an innovative way***. Proceeding from this, the authors at the previous stage of development elaborated the concept of creating an Automated System for Controlling the Modes of electric current treatment of the melt (ASC-MECT), embodied in the scheme of an integrated three-component information system **(ITIS)** [7]. The main functional operations of the algorithmic paradigm of ITIS are envisaged to be implemented with the use of the software of the computer modeling block (BCM) integrated into **ITIS**. BCM should provide the formation of numerical layouts of the structure formation mode and the selection of prognostic archetypes [7], with the use of actual (empirical) data on the structure of treated samples of castings accumulated in ITIS in the specialized library of templates structure (L-TS). It is this procedure that determines the success of solving the problem of purposeful formation of quality indicators of cast products.

Therefore, to mathematical models and algorithms for their numerical implementation, which are intended for this purpose, the special features should be required, both in terms of the accuracy and rate of solutions convergence, along with the versatility of simulated objects configurations, as well as the physical adequacy of the computational problem statement and the interpretation of the results obtained. Obviously, the fulfillment of such requirements cannot be provided with a single type of computer models, taking into account the interdisciplinary content of modeling tasks. This will necessitate a certain set (package) of computer models (SUCM), unified by physical identifiers and scale factors and united by a common data exchange protocol. At the same time, the SUCM should have a sufficiently *flexible structure* that makes it possible to adapt conveniently the models to the of simulation conditions of any specific processing modes and the formation of numerical layouts of the structure formation process within the framework of a single algorithmic scheme.

In such aspect the computer model at a level of software realization can be represented as an algorithmic pattern-matrix or package of patterns (PPCM) and systematized set of specialized software modules (SSSM), which, in accordance with specified conditions of the model problem, are coupled with a matrix. Each specialized module should ensure the implementation of a specific set of mathematical operations, which corresponds to the model problem. Such **an innovative approach** to the construction of SUCM will allow the possibility of further improvement and expansion of the of model problems range from the very beginning.

The currently known computer models that are used to calculate ESO processes cannot fully meet the specified requirements due to certain limitations of the range of model problems associated in fact with the same circumstance: with all the variety of real physical conditions, their solution is reduced practically to a single mathematical scheme, i.e. partial differential equations (PDEs) of field theory. Their numerical solution is performed mainly by finite element methods

(FEM), for which typical software packages, such as ANSYS or COMSOL, are used.

The experience gained in numerical modelling of ECT processes based on PDE-FEM, including that obtained by the authors, shows that when they are used for practical ECT problems, a number of disadvantages and limitations appear. Some of them are inherent to the numerical methods themselves, while others are due to the peculiarities of their application to ECT problems. Therefore, simulation results in many cases may not adequately reflect real physical phenomena. Consequently, in such a situation, there is hardly any reason to expect the construction of a universal computer model that covers the whole variety of multiphysics phenomena of ECT.

Taking these circumstances into account, the authors turned to alternative form of the same ECT tasks, to which the PDE-FEM method is applied, by way of integral equations (IE) [10]. Integral equations are equivalent to PDE in mathematical content, but in terms of computational properties they have a clear advantage over them in the corresponding class of problems [11, 12]. However, it should be noted that, as against the PDE-FEM method, for use of the IE method, there are currently no sufficiently developed application packages suitable for the numerical solution of various physical problems of the ECT. To make up for their absence and create the prerequisites for the implementation of the tasks outlined in the above-mentioned concept of ASC-MECT, the authors, on the basis of the canonical forms of IE of ECT processes, have elaborated a universal format of computer models suitable for design of applied programs and use in algorithms for controlling the modes of electric current processing of the melt, which is described in [11]. This development [11] formed the basis for the presented in this work an innovative ***system of computer modeling*** of ECT processes, which is built on the above-mentioned pattern-modular principle.

When constructing this system, the authors were guided by the methodological principles that are laid down in the classification of interdisciplinary multiphysics problems [8, 9]. Firstly, complex multiphysical ECT problems are subjected to decomposition into simpler monophysical (model) tasks, defined in their partial domain [9], and a step-by-step numerical solution. Secondly, at each subsequent stage of the specific monophysical tasks formulation, it should be ensured that the output and input data of individual tasks are conjugated in time in accordance with the logic and order of the multiphysical processes of the ECT.

Perceiving the above classification as a productive basis, the authors relate it to the highest level of systemic attributes hierarchic structure of the ECT model tasks (MT) set. However, considering the variety of melt ECT modes controlling tasks according to the quality criteria of the casting structure envisaged by **ITIS** algorithmic paradigm, it seems necessary to introduce an in-depth systematization (taxonomy) of the characteristic features of their totality [13], specified for each model problem. According to the taxonomy of the MT, there is need to systematize the entire range of computer models of ESP processes integrated into **ITIS**, taking into account the requirements that are imposed on the SUCM in terms of the mathematical forms of the initial equations and algorithmic procedures for their numerical solution. In connection with the above, it turns out to be advisable to draw up such a classification also with respect to indicators that reflect the results of modeling, i.e. a taxonomy of numerical layouts of ECT modes (NLM) based on generalized quantitative estimates of the intensity of energy impacts (GQEI) [7].

Based on the above considerations, the authors set the purpose of this paper as follows.

The purpose of the paper is to develop compiling principles and to device an innovative pattern-modular ***system of computer modeling*** of ECT processes, its mathematical tools and software for solving problems of melt ECT modes controlling, based on formalized integral equations of multiphysical processes.

In order to achieve the objective, the following tasks need to be solved:

a) elaborating the structure and function scheme of the system of computer modeling of ECT processes (SCM-ECT);

b) systematizing the monophysical components of the model tasks set and generalized quantitative estimates of intensity GQEI of energy impacts;

c) developing the set of unified computer models SUCM in the form of algorithmic patterns PPCM with a set of specialized software modules SSSM to them.

The basics of compiling the SCM-ECT. The combination of the above arguments justifies the necessity of setting a multifaceted problem that is creating a computer modeling system according to the functional objectives of **ITIS** as a part of ASC-MECT. Considering the outlined problem in the unity and integrity of all its components, the authors present SCM-ECT (hereinafter abbreviated as "SCM") as a set of software tools (algorithmic units), the general structure of which is shown in the diagram Fig. 1. The functions of SCM are implemented by the algorithmic units represented on it, which provide:

- setting conditions and initial data of model tasks according to their classification (SCID-MT unit);
- defining (identifying) the mathematical implements and algorithms for numerical solution of the corresponding task, which realize the assignment of SUCM (IMTA-SUCM unit);
- composing the unified arrays of NLM-GQEI, obtained from modeling results (CUA-NLM unit);
- unit for introducing the unitized data exchange protocol(UDEP), unified for all program modules by physical identifiers, scale factors and program formats.

One of the most important factors in ensuring the operability of such a complex system is the orderliness and clear addressing of unified data flows and their adequate interpretation.

Consequently, to implement the mentioned data exchange protocol, it is necessary to introduce a concise intrasystem *pseudolanguage*, that is a local terminological environment ("formal explicit descriptions of the subject area terms and relations between them") or *ontology* [14].

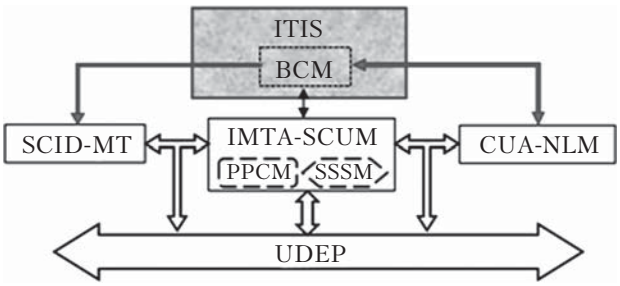


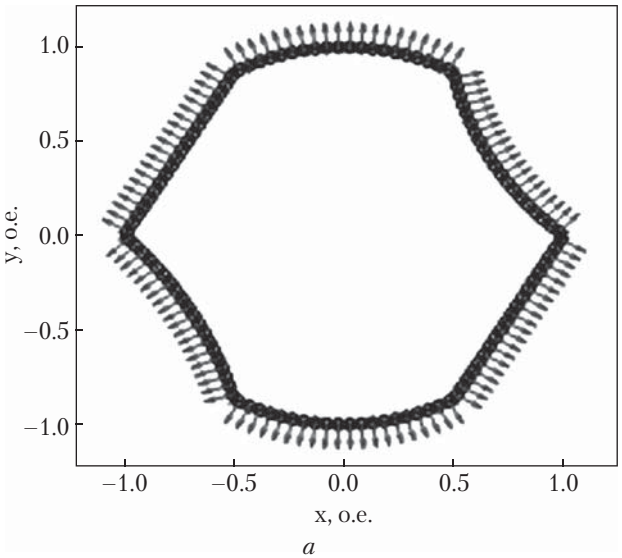
Fig. 1. *General structure of SCM*

An objective precondition for the introduction of a specialized ontology in SCM is the similarity of the mathematical description and algorithms of the solution of many model problems of ECT, from which follows the possibility and expediency for applying the principle of formalization of the intrasystem procedures description in ontological categories. Thus, the specified ontology will be a means of providing functional links (data exchange procedures) in SCM. To explain the way of introduction and use of such a "custom" ontology, it is better to consider an apparent demonstrational example for conditional but typical task.

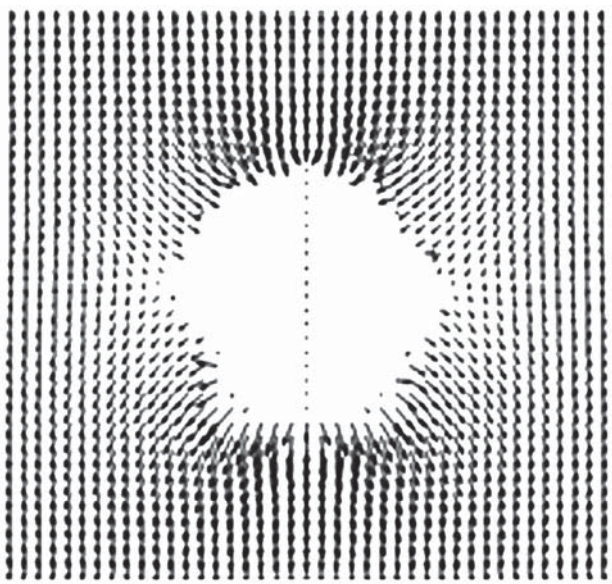
Demonstrational example: in 2D space, in a uniform electrostatic field of a given intensity $\boldsymbol{E}^{(0)}$ a conducting body with an arbitrary boundary contour L is placed (Fig. 2, *a*). The task is to calculate the resultant field $\boldsymbol{E}$. Such a field is shown in Fig. 2, *b*, with its calculation further explained.

In a conducting medium, as it is known, there is no electrostatic field, then the above statement of the problem corresponds to the boundary conditions of the external Dirichlet problem (the first boundary value problem), the solution of which is sought in the form of the potential u of a double layer of charges distributed along the contour L with a density ν [10]. In this case this problem is satisfied by an integral equation of the form:

$$\nu(P)-\frac{1}{\pi}\oint_L \nu(M)\frac{\partial}{\partial n_M}\ln\frac{1}{r_{PM}}dl_M = u^{(0)}\Big|_L(P), \quad P\in L, \quad (1)$$



a



b

Fig. 2. Distribution of normals on the contour (*a*) and vectors of field strength ***E*** *(b)*

where

$$r_{PM} = \sqrt{\left(x_P - x_M\right)^2 + \left(y_P - y_M\right)^2}$$

is the radius-vector drawn from the integration point M on the boundary surface (contour) L to any observation point P on the same surface, $\overline{n}_M$ is the normal to the contour L at the integration point, and $u^{(0)}$ is the potential given by boundary conditions.

However, in this case there is an essential peculiarity of the problem conditions: since the external surface of the conductor is a zero equipotential, the right part of this equation $u|_L = 0$, so it becomes homogeneous and has only a trivial (zero) solution. Then the mathematical description of the problem should be reformulated by taking as the basis the third Green's formula for the external problem potential [10] that is expressed through the potential of a simple layer. Taking the derivative of the function $u(P)$ along the normal to the boundary surface (denote it by $\partial u/\partial n = -E_n = \sigma$), taking into account the jump of the derivative of the simple layer potential on the boundary [10], we obtain a simple integral equation from those that are covered by the system of equations for the general case in [11].The found equation corresponds to the formulation of the problem of finding the density of secondary sources σ on the interfaces between media according to the Greenberg method [15]:

$$\sigma(P) = 2\varepsilon_0\lambda\left[E_n^{(0)}(P) + \frac{1}{2\pi\varepsilon_0}\oint_L \sigma(M)\frac{\partial}{\partial n_P}\ln\left(\frac{1}{r_{PM}}\right)dl_M\right], \quad (2)$$

where $E_n^{(0)}$ is the normal component of the electric field strength set on the boundary surface; ε_0 is dielectric constant.

The kernel of integral operator in IE (2), inherent in the potential of a simple layer, has the form:

$$K(P,M) = \frac{\partial}{\partial n_P}\ln\left(\frac{1}{r_{PM}}\right) = \frac{\cos(\overline{r}_{PM}, \overline{n}_P)}{r_{PM}}, \quad (3)$$

where $\overline{n}_P$ is the normal to the contour L at the observation point; it differs from the kernel of IE (1) in that the derivative is taken at the observation point, not at the integration point.

In so doing, the correct calculation of the distribution of normals along the contour is extremely important for a clear numerical reproduction of the fundamental mathematical properties of kernels of type (3). Therefore for selected example the distribution of normals calculated with the use of the special algorithm named “geometrical

platform" (GP) [16] developed by the authors is shown directly on the contour in Fig. 2, *a*.

The coefficient

$$\lambda=\frac{\varepsilon_i-\varepsilon_e}{\varepsilon_i+\varepsilon_e}$$

is a factor of difference in the electrical properties of the media: ε_i is dielectric permeability of the internal volume (*i*) of the body, and ε_e is permeability of the external medium (*e*). At their interface, there is a jump in the normal component of the field strength vector, which causes the appearance on the boundary surface of a bound charge distributed over the surface with a density σ:

$$\varepsilon_0(E_{ne}-E_{ni})=\sigma\,. \qquad (4)$$

So the resulting field at any point *Q* of the entire space is defined as the sum of the fields of primary and secondary sources:

$$\boldsymbol{E}=\boldsymbol{E}^{(0)}+\boldsymbol{E}^{(\sigma)}, \qquad (5)$$

where the field of bound charges

$$\boldsymbol{E}^{(\sigma)}(Q)=-grad_Q\frac{1}{2\pi\varepsilon_0}\oint_L\sigma(M)\ln\frac{1}{r_{QM}}dl_M\ , \qquad (6)$$

is the potential gradient of a simple charge layer σ in 2D space [15].

However, in our example, the field inside the conducting body is absent, then according to (4)

$$\boldsymbol{E}_i=0,\ \text{a}\quad \sigma=\varepsilon_0E_{ne}\,, \qquad (7)$$

which corresponds to the case when $\varepsilon_i\to\infty$, and, accordingly, $\lambda\to 1$.

It is known that the solution of equations of the form (2) is carried out by approximating the integral whith a finite sum and reducing the IE to a system of linear algebraic equations (SLAE), the solution of which can be obtained by various methods, in particular, successive approximations (iterations). The results of such a calculation for the given example are shown in Fig. 2, *b* in the form of a vector field of strength ***E***.

At the same time, the stated model for solving the direct problem (the body is in the field of external sources) also has an inverse statement, equivalent to the shielding problem, in which the primary sources of the field are located in the cavity of a massive (thick-walled) of a conductive body of infinite thickness. The IE for such a problem remains the same as (2), the only difference is that the direction of the normal vector changes to the opposite, because the space of the cavity becomes the external region (*e*), while the massive body becomes the internal one (*i*).

To perform numerical calculations, the transition from the direct problem to the inverse problem does not encounter any difficulties, as the only necessary thing is to change the direction of the contour *L* from positive (counterclockwise) to reverse (clockwise). In the mentioned GP algorithm, such a procedure is carried out at the stage of setting the contour parameters. Figure 3b shows a map (topography) of the equipotentials of the field excited by two electrodes in the cavity in Fig. 3, *a* of the same shape as the contour in Fig. 2, *a*, that was calculated according to the described model.

The given example (Figs. 2—3) reveals an important method-logical fact: the structure of the mathematical description of a large group of boundary value problems of field theory, different from each other, is actually identical, because it represents the Fredholm integral equation [10] of the second kind for potentials of simple and double layer of charges with allied kernels. The calculation of these kernels is based on the same "GP" algorithm for calculating the spatial parameters of the boundaries of the computational domains. Moreover, in the ECT processes, as already noted, physical phenomena of different scale arise from the field of heat transfer, hydrodynamics, acoustics, etc., mathematical models of which are quite similar to the above problems, and in total they constitute quite a significant set.

This fact clearly indicates that there are compelling objective prerequisites for formalization and automation of procedures for mathematical description and solving problems of this class. However, it is obvious that each separate task from this set has individual specifics and a lot of features that distinguish them from each other in the parametric formats of physical identifiers. In

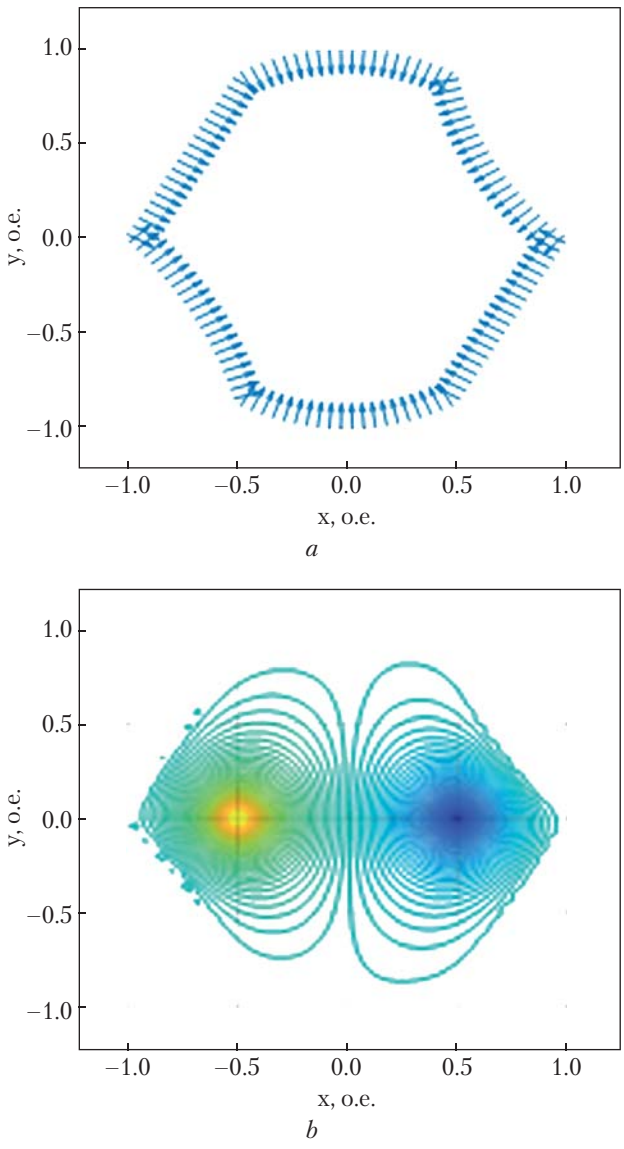


Fig. 3. Distribution of normals (*a*) and equipotentials (*b*) in the internal problem

such conditions, it becomes necessary to create a certain unified algorithmic platform (pattern) in order to compose, on its basis, specified computer models of particular problems of simulation of ECT modes from autonomous program blocks. For this, in the structure of the SCM (Fig. 1), a block of algorithmic patterns PPCM with a corresponding set of specialized software modules SSSM is provided.

However, it should be noted that due to significant diversity in the architecture of global (object) programming and local (operational) manipulations for procedures of composing models of particular tasks in the format of a unified pattern, the problem of their terminological coupling becomes critical [14], that is, the construction of the very ontology, which, according to the stated principle of organization of functional connections in the SCM, is defined as a linguistic tool for ensuring the procedures of data exchange and transfer of information arrays (information packages or IP).

Systematization of model problems, computer models and numerical layouts of ECT modes. As the specified ontology it seems expedient to use the mentioned taxonomy of characteristic features of model problems of ECT and computer models (CM), which is based on the connection between the phenomenological interpretation of ECT processes, their mathematical models and computational algorithms. On the grounds of the analysis of this connection content, the authors defined the systemic categories of the mentioned ontology, taxonomy classification attributes [13] and principles of MT attributes codification in the algorithmic environment of SCM. According to these principles the taxonomic codifier (TC) called *Takstrum* that is presented below has been compiled.

By codifying the characteristic features of MT as system (classification) attributes of TC, which determine the disposition of modeling, the implementation of functional connections between modules in SCM is ensured. The introduction of such codification is similar to the synthesis technique for a computational library of modeled objects masks, used in [17] for analogous purposes. So, methodological sense of introduction of TC is that its attributes identify the CMs that are adequate for a certain MT, and incorporate them into the **ITIS** algorithmic environment using software (protocols)of data exchange with BCM, where NLM are formed. Thus, in the entire set of multiphysics process of ECT modeling tasks, each par-

tial task receives its unique code in the categories of MT attributes codifier, which becomes a key for compiling a particular CM of prognostic archetype and numerical layout of structure formation in a given mode of electrocurrent melt treatment.

The repertory of the classification attributes, systematized according to the categories of MT attributes, forms the structure of TC, adapted for the solution of SCM-ECT tasks. It consists of four profile arrays-attributives that are connected by causal relations: AMT means attributive of model tasks of ECT; AMI means attributive of mathematical implements; ACP means attributive of computational procedures of CM, and ANLM-GQEI means attributive of unified arrays of numerical layouts of ECT modes and generalized quantitative estimates of intensity of energy influences. The specified attributes serve as operational means, which in the coded form embody the logical links of data transmission channels according to the scheme of general structure of SCM, shown in Fig. 1. At that, AMT-attributive is an accessory of the SCID-MT algorithmic unit, AMI- and ACP-attributives are ones of the IMTA-SUCM unit, and ANLM-GQEI attributive is an accessory of the FUA-NLM unit.

Attributives of *Takstrum* codifier. The explanation of the principles of codification laid down in *Takstrum*, the description of its components and the characteristic of links between them is appropriate to give with corresponding references to the example of conditional task, which was considered earlier.

1) *AMT attributive*. The composition of this attributive is formed on the basis of the analysis of physical factors (PF) that determine the content of the model problem. Its purpose is to provide a clear identification of MTs, to determine the conditions of existence and interaction of modeling objects in the environment through the parameters of spatial location of computational segments of the object and temporal parameterization of related processes duration.

The codification of the characteristic features of MT by the AMT-attributive is built on a two-level principle in the form of a matrix Amodtask = = [A1, A2, ..., A6], where the designations of the elements |A1, A2, ..., A6| are a cipher of the categories into which homogeneous PFs are grouped. In turn, each of these elements is a linear matrix of attributes codes of the corresponding category.

Below, in Table 1, the content of the PF categories is given and the codes of their attributes are presented.

A1 — kinds of primary physical fields that determine the statement of the partial MT of ECT.

A2 — types of boundary value problems that determine the boundary conditions for the equations corresponding to the mathematical formulation of the MT.

A3 — types of material objects exposed to the physical fields in the MT.

A4 — types of impact that the field exerts on material objects: structural and force.

A5 — coordinate metrics and spatial parameters that determine the statement of the partial MT.

A6 — interval-time parameterization or the type of process that determines the statement of MT.

The taxonomic cipher of individual MT is formed by assigning to elements of the matrix Amodtask (A1, .., A6) a numerical code of features that identify the task according to Table 1.

Thus, the direct problem from the given demonstrational example (the "Demo" task), which refers to static first internal boundary value problem for an electric field in a homogeneous medium without physical influences in 2D Cartesian coordinates, should be given by the following code:

A1 = 001; A2 = 001∪0; A3 = 001; A4 = 010;

A5 = 001; A6=001 (where ∪ is disjunction);

or: Amodtask = [001, **001∪0**, 010, 010, 001, 001].

Accordingly, for the inverse (external) coding problem will take the form:

Amodtask = [001, **001∪1**, 010, 010, 001, 001].

2) *AMI attributive*. The attribute codes of mathematical implements of partial model tasks AMI are given in Table 2. They are built, as for AMT, in the form of a matrix of categories

B = [B1, ..., B4]:

B1 — mathematical forms of sources creating the primary field that define the boundary conditions.

B2 — kinds of kernels of integral operators, which define the global action of field sources.

B3 — types of derivatives of integral operators.

B4 — localized (grid) forms of operations of numerical differentiation and integration.

In particular, for the "Demo" task, this attribute will take the following form:

Bmattool (B1, B2, B3, B4) =

= Bmattool [010, 010, 001∩ 011, 011],

where B1 = 010; B2 = 010; B3 = 001∩11; B4 = = 011; (∩ is conjunction).

3) *ACP attributive* of categories of computational procedures.

Table 1. **Categories and Attributes of Physical Factors That Determine the Formulation of the Model Problem**

Categories	A1	A2		A3	A4	A5*	A6*
Code	Content of attribute						
001 U0	Electric field	1st boundary	internal	Homogeneous medium	Heat generation	Cartesian in 2D	Static
001 U1			external				
010 U0	Current field	2nd boundary	internal	Heterogeneous medium	Variable medium parameters	Cartesian in 3D	Quasi-stationary
010 U1			external				
011	Magnetic field	3rd boundary		Solid state (one body)	Mechanical forces	Cylindrical in 2D	Discrete
100	Thermal field	Hybrid boundary		Several bodies system **)	Local deformation	Cylindrical in 3D	Transitional
101	Hydrodynamic field	Secondary sources in a closed area		Composite system	Motion and flow	Spherical parameters	Stochastic

*) Together with the definition of a specific feature code of the corresponding category, a full array of given numerical values of the model parameters in the format of the used software product is supplied.

**) Multi-connected area with separated boundaries.

Table 2. **Categories and Attributes of Mathematical Implements of Partial Model Tasks**

Category	B1	B2	B3	B4
Attribute code	Content of attribute			
001	Localized charges, dipoles and currents	Scalar 3D potentials	Spatial derivatives of scalar potentials	Numerical integration over area and volume
010	Simple and double layers of charges	Scalar 2D potentials	Spatial derivatives of vector potentials	Numerical integration along lines and surfaces
011	A simple layer of currents	Vector 3D potentials	Normal derivatives of scalar potentials	Difference spatial gradient and divergence
100	Volume distribution of charges and dipoles	Vector 2D potentials	Normal derivatives of vector potentials	Difference spatial rotor
101	Volume current distribution	Time derivatives scalar potentials	Tangent derivatives of scalar potentials	Difference spatial Laplacian
110	–	Time derivatives of vector potentials	Tangent derivatives of vector potentials	Difference surface gradient and divergence

C1 — the formation of arrays of reference points for discretization of computational domains from A3 according to the conditions from A5 (Table 1).

C2 — the calculation of local geometric parameters of discrete elements (DE) of computational domains.

C3 — the calculation of the values of operators from B2 (Table 2) for DE based on data from C1 and C2 and the formation of SLAE components matrices that approximate the integral equations system of MT.

C4 — the procedures for solving SLAE and obtaining the indices of solution quality.

For the same "Demo" example, the AOP attribute will gain the following form:

Ccalctool (C1, C2, C3, C4) =

= Ccalctool [001, 001, 010, 100].

The presented tables of the ordered attributes of information arrays, handled during the modeling of ECT processes, provide an adequate conversion of data packages in appropriate formats when they are transferred to the corresponding software modules and the construction of pass-through computational procedure at the output of which data arrays are formed for synthesis in ITIS of protocols of guided commands regarding a mode of technological operations of processing. For this purpose, the arrays of initial data are codified by the ANLM-GQEI attributive according to the same principle as previous ones.

4) *ANLM-GQEI attributive* of numerical layouts of ECT modes and generalized quantitative estimates of the intensity of energy impacts [7]. This attributive is closely related to the quality indicators of castings structure, which are determined by the results of experimental studies and accumulated in the library of structure templates, which is the part of ITIS. Since experiments on the study of the linkage between internal phenomena in ECT processes and their consequences are ongoing, it is premature to define a detailed list of attributes of GQEI, but in general terms, the nature of the categories of estimates that should be applied preliminary may be already specified.

They are listed below.

S1 — spatial distribution of current density and physical fields covered by category A1 according to source type from B1.

S2 — localization and distribution of effects specified in category A4.

S3 — integral estimates of the energy parameters of the ECT stationary modes from categories A6.

S4 — estimates of temporal characteristics of integral parameters of nonstationary modes from A6.

The codification of the attributes of the given categories will be formed as the library L-TS is filled.

Thus, the complete suite of linkage logical units of SCM algorithmic modules for construction of pass-through computational process of solving ECT model tasks is formed.

The diagram of SCM-ECT operation. According to categories of information packages, which are defined by the corresponding attri-

Table 3. **Categories and Attributes of Computational Procedures**

Categories	C1	C2	C3		C4
Attribute code	Content of attribute				
001	Arc discrete elements GP	Complex shape of arc elements	Matrix calculation	Square matrix of coefficients	Direct methods
010	Boundary finite elements (BFE)	Polynomial Approximation of BFE		Regularized square matrix	Decomposition of matrices
011	Parametric algorithms	Analytical geometry formulas	Routine arithmetic calculations	Band matrix of coefficients	Simple iterative methods
100	Projective algorithms	Projective image data (drawings)		Block-diagonal matrices	Iterations with regularization

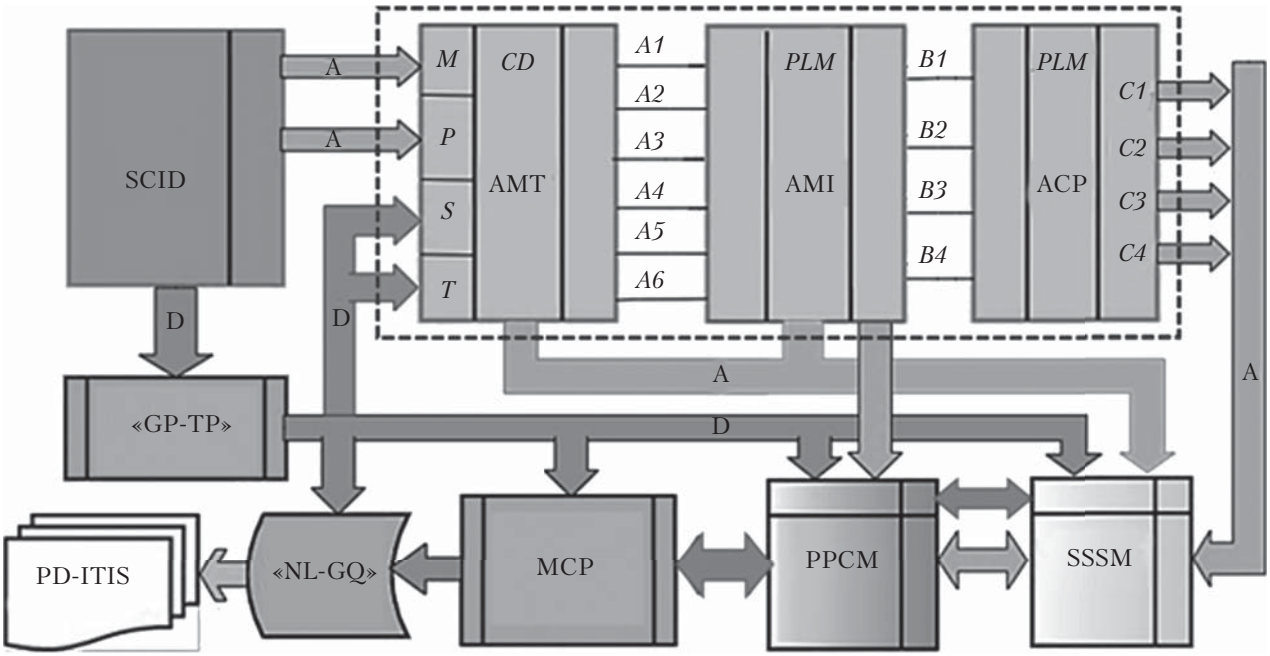


Fig. 4. Functional diagram of SCM-ECT: SCID-unit for setting conditions and initial data of model tasks; GP-TP — an autonomous processor GP-TP; AMT — the codifier of the physical factors defining MT; AMI — the codifier of mathematical implements of MT; ACP — the codifier of computational procedures; SSSM — a set of specialized software modules; PPCM — a package of patterns of CM; GOP — the main computing processor; NL-GQ — local processor of NLM-GQEI data; PD-ITIS — protocols of NLM-GQEI data transmitted to ITIS

butes, and the general structure of SCM, given in Fig. 1, the sequence of process stages of computer modeling of ECT partial tasks should be represented by the functional diagram shown in Fig. 4. In this scheme, an analogy is used with the graphic symbolism of the elements of microprocessor circuits, with the device of which the described SCM has a substantial similarity. The dotted line on the diagram indicates the structure of the codifier *Takstrum*.

The system works as follows.

The set of data, formed in the above mentioned information system IT IS that gives a description of the partial MT statement, is loaded to SCID-unit (conditions and initial data of MT). In this unit, indicated data are divided into four logical-semantic groups:

(*a*) of mathematical forms (index M means "Math.") and (*b*) of physical characteristics (P means "Physics"),

(*c*) of spatial configuration parameters (S means "Space") and (*d*) of temporal format (T means "Time").

The first two groups contain static data that define invariable conditions of a particular MT, and have a content-attributive character. However, the other two groups reflect the variation aspects of the problem in the quantitative-numerical format. All groups of data are transmitted to the first stage codifier (AMT-block) through separate information channels (buses): M and P types — through analogue (text) buses denoted by "A"; and S and T types — through digital buses denoted by "D".If "M-P" data are transferred to AMT-block directly in the form of introduced ontological lexemes, "S-T" data preliminarily come to autonomous processor block "GP-TP" for preparation of the numerical basis of MT. In this processor, with the use of the "geometric platform" (GP) algorithm [16],

the geometric characteristics of the simulated objects necessary for the formation of IE are calculated, and the parameters of time projections (TP) for the calculation of time derivatives of physical variables are determined. In the AMT-block that is represented as a programmable microprocessor (*CD*-module), the packages of task unified parameters is formedin the format of input signals — ontological lexemes. This block performs the function of an encoder and generates the cipher of MT features — array Amodtask that is fed to the input of the second stage of the codifier — AMI-block represented as programmable module *PLM*. It identifies adequate mathematical tools and generates the output code package Bmattool. The indicated signal is fed, firstly, to the *PLM*-module PPCM, where the composition of algorithmic patterns of synthesized CM is defined; secondly, according to the specified code in the ACP-block (*PLM*-module), the package Ccalctool is formed. It is transmitted to the module SSSM, where specialized software modules (SSM) corresponding to certain MT features have been searched/selected. The selected SSMs are translated to block PPCM for conjugation with certain CM patterns. The CM synthesized in this way is loaded to the main computing processor (MCP), where calculations are performed according to algorithms embedded in the patterns. The results obtained are transmitted to the local processor "NL-GQ" in which the NLM-GQEI data protocols are formed, which are then used in ITIS.

Note that actually the implementation of the above process on the basis of existing microprocessor elements is purely conditional, since it requires more powerful computing tools, but in fact they should be embodied in the algorithmic equivalent of the presented microprocessor chart.

Patterns of PPCM and their application. The patterns are unified abstract forms for composing algorithmic procedures of solving the particular MTs. In accordance with the logical structure of CM, patterns should be divided into two types: structural and procedural.

1) *Structural patterns* are matrix forms, ordered as sets, in which it is rightful to use the operations attach to this category of mathematical objects [18]. Patterns serve as a tool for performing computational procedures stipulated by these methods, with the use of software modules selected in the SSSM block with a batch of MT features that are given by the codifier.

According to the content of these algorithms, these batches form the patterns of two levels. Their content is reflected by the expressions below. The pattern of both levels are formatted arrays of numerical data that determine the spatial distribution of primary and secondary sources of fields, calculated in the GP-TP processor.

A. Patterns of the first level P1 are represented by expression (8) and generated as arrays of geometric parameters of points or elements of discretization in areas where field sources are localized, as well as in areas of calculation of the sought functions. The patterns are formed as column matrices according to the "nest" principle: each discrete element (DE) of the field distribution area corresponds to its own "nest" that is a separate low-dimensional array in which its local spatial characteristics are laid down. The format of such an array is defined solely by the convenience for manipulation in the program code. Thus, in the notation (8), the expression for the pattern $\boldsymbol{P}$ means that it is referred to the boundary domain $\boldsymbol{S}$ where the given integral equation of MT is defined. The pattern has dimension m that indicates the number of DEs of the integral operator. The "nests" of the pattern $\boldsymbol{p}_i = [\overline{r}_i, \overline{n}_i, \overline{c}_i]$ contain: $\overline{r}_i$ is vector of DE coordinates according to attribute A5; $\overline{n}_i$ is vector of DE normal parameters; $\overline{c}_i$ is vector of DE curvature parameters.

$$\boldsymbol{q}_h = [\overline{\rho}_h, \overline{\nu}_h, \overline{\chi}_h], \boldsymbol{q} \in \boldsymbol{Q}\big|_{\dot{A}} : \; h = 1, ..., k$$

$$\boldsymbol{p}_i = [\overline{r}_i, \overline{n}_i, \overline{c}_i], \boldsymbol{p} \in \boldsymbol{P}\big|_S : \; i = 1, ..., m$$

$$\boldsymbol{z}_j = [\overline{\xi}_j, \overline{\theta}_j, \overline{\kappa}_j], \boldsymbol{z} \in \boldsymbol{Z}\big|_V : \; j = 1, ..., n$$

where

$$\boldsymbol{Q}=\begin{pmatrix}[\overline{\rho}_1,\overline{\nu}_1,\overline{\chi}_1]\\ \ldots\ldots\ldots\\ [\overline{\rho}_h,\overline{\nu}_h,\overline{\chi}_h]\\ \ldots\ldots\ldots\\ [\overline{\rho}_k,\overline{\nu}_k,\overline{\chi}_k]\end{pmatrix};\ \boldsymbol{P}=\begin{pmatrix}[\overline{r}_1,\overline{n}_1,\overline{c}_1]\\ \ldots\ldots\ldots\\ [\overline{r}_i,\overline{n}_i,\overline{c}_i]\\ \ldots\ldots\ldots\\ [\overline{r}_m,\overline{n}_m,\overline{c}_m]\end{pmatrix};\ \boldsymbol{Z}=\begin{pmatrix}[\overline{\xi}_1,\overline{\zeta}_1,\overline{\theta}_1]\\ \ldots\ldots\ldots\\ [\overline{\xi}_j,\overline{\zeta}_j,\overline{\theta}_j]\\ \ldots\ldots\ldots\\ [\overline{\xi}_n,\overline{\zeta}_n,\overline{\theta}_n]\end{pmatrix}. \tag{8}$$

The pattern $\boldsymbol{Q}$ of dimension k, referred to the domain $\boldsymbol{A}$, where the distribution of primary sources (for example, charges) is given, and the pattern $\boldsymbol{Z}$ of dimension n, assigned to the domain $\boldsymbol{V}$, where the values of the sought functions (induced fields) should be calculated, are constructed in quite a similar way. Accordingly, in the "nests" $\boldsymbol{q}_h$ the vector contains coordinates of the sources, reflects specific data on their properties, assigns the parameters of the sources intensity, and in the "nests" $\boldsymbol{z}_j$ the elements of array also reflect the corresponding properties of the sought functions.

B. Patterns of the second level P2 are 2D sets of geometric parameters combined from the elements of the sets P1, prepared for direct use in calculations of two-point operators of such a type as the kernel of the IE of demo example, in particular, for calculating the right-hand sides of the SLAE, which approximate the mentioned integral equations. Patterns P2 are formed by direct (Cartesian) multiplication of two sets [18] from the content of P1 and presented in expressions (9). Their dimension is defined by the dimensions of the factors:

$$\boldsymbol{B}=\boldsymbol{Q}\times\boldsymbol{P}=\left\{(\boldsymbol{q},\boldsymbol{p})\middle|\boldsymbol{q}\in\boldsymbol{Q}\cap\boldsymbol{p}\in\boldsymbol{P}\right\}\Rightarrow$$
$$\Rightarrow\boldsymbol{b}_{h,i}=\left(\boldsymbol{q}_h,\boldsymbol{p}_i\right),\boldsymbol{b}\in\boldsymbol{B}\Big|_{C\mapsto S}; \tag{9a}$$

$$\boldsymbol{D}=\boldsymbol{P}_M\times\boldsymbol{P}_P=$$
$$=\left\{\left(\boldsymbol{p}_\upsilon,\boldsymbol{p}_i\right)\middle|\boldsymbol{p}_\upsilon\in\boldsymbol{P}_M\cap\boldsymbol{p}_i\in\boldsymbol{P}_P\right\}\Rightarrow \tag{9b}$$
$$\Rightarrow\boldsymbol{d}_{\upsilon,i}=\left(\boldsymbol{p}_\upsilon,\boldsymbol{p}_i\right),\boldsymbol{d}\in\boldsymbol{D}\Big|_{S\mapsto S}.$$

In expanded form, the patterns $\boldsymbol{B}$ and $\boldsymbol{D}$ are given in expression (9c), they constitute a geometric basis for calculation of the values of integral operators acting from points of one area to points of another area ($\tilde{\boldsymbol{N}}\mapsto\boldsymbol{S}$), that is, in fact, they represent the "influence functions". In particular, the pattern B corresponds to the "influence" of the of primary sources distribution area $\boldsymbol{A}$ on the boundary surface of the simulated object $\boldsymbol{S}$. However, template $\boldsymbol{D}$ contains the geometric basis of the mutual influence of secondary sources, distributed in the area $\boldsymbol{S}$ ($\boldsymbol{S}\leftrightarrow\boldsymbol{S}$).

$$\boldsymbol{B}=\begin{pmatrix}(\boldsymbol{q}_1,\boldsymbol{p}_1)\ldots,(\boldsymbol{q}_h,\boldsymbol{p}_1)\ldots,(\boldsymbol{q}_k,\boldsymbol{p}_1)\\ \ldots\ldots\ldots\ldots\ldots\\ (\boldsymbol{q}_1,\boldsymbol{p}_i)\ldots,(\boldsymbol{q}_h,\boldsymbol{p}_i)\ldots,(\boldsymbol{q}_k,\boldsymbol{p}_i)\\ \ldots\ldots\ldots\ldots\ldots\\ (\boldsymbol{q}_1,\boldsymbol{p}_m)\ldots,(\boldsymbol{q}_h,\boldsymbol{p}_m)\ldots,(\boldsymbol{q}_k,\boldsymbol{p}_m)\end{pmatrix};$$
$$\boldsymbol{D}=\begin{pmatrix}(\boldsymbol{p}_1,\boldsymbol{p}_1)\ldots,(\boldsymbol{p}_\upsilon,\boldsymbol{p}_1)\ldots,(\boldsymbol{p}_m,\boldsymbol{p}_1)\\ \ldots\ldots\ldots\ldots\ldots\\ (\boldsymbol{p}_1,\boldsymbol{p}_i)\ldots,(\boldsymbol{p}_\upsilon,\boldsymbol{p}_i)\ldots,(\boldsymbol{p}_m,\boldsymbol{p}_i)\\ \ldots\ldots\ldots\ldots\ldots\\ (\boldsymbol{p}_1,\boldsymbol{p}_m)\ldots,(\boldsymbol{p}_\upsilon,\boldsymbol{p}_m)\ldots,(\boldsymbol{p}_m,\boldsymbol{p}_m)\end{pmatrix} \tag{9c}$$

By full analogy with pattern $\boldsymbol{B}$, the "influence" patterns ($\boldsymbol{A}\mapsto\boldsymbol{V}$) and ($\boldsymbol{S}\mapsto\boldsymbol{V}$) are built:

$$\boldsymbol{\Gamma}=\boldsymbol{Q}\times\boldsymbol{Z}=\{(\boldsymbol{q},\boldsymbol{z})|\boldsymbol{q}\in\boldsymbol{Q}\cap\boldsymbol{z}\in\boldsymbol{Z}\}\Rightarrow$$
$$\Rightarrow\boldsymbol{\gamma}_{h,j}=(\boldsymbol{q}_h,\boldsymbol{z}_j),\boldsymbol{\gamma}\in\boldsymbol{\Gamma}|_{A\mapsto V};$$
$$\boldsymbol{\Omega}=\boldsymbol{P}\times\boldsymbol{Z}=\{(\boldsymbol{p},\boldsymbol{z})|\boldsymbol{p}\in\boldsymbol{P}\cap\boldsymbol{z}\in\boldsymbol{Z}\}\Rightarrow \tag{9d}$$
$$\Rightarrow\boldsymbol{\omega}_{i,j}=(\boldsymbol{p}_i,\boldsymbol{z}_j),\boldsymbol{\omega}\in\boldsymbol{\Omega}|_{S\mapsto V}.$$

So, the structure of the patterns $\boldsymbol{\Gamma}$ and $\boldsymbol{\Omega}$ is quite obvious from the above considerations, it coincides with the structure of the pattern $\boldsymbol{B}$, so it is not necessary to note down them in form (9c).

Thus, the created forms $\boldsymbol{B}$, $\boldsymbol{D}$, $\boldsymbol{\Gamma}$ and $\boldsymbol{\Omega}$ constitute the complete suite of patterns that set the geometric basis for calculating integral operators in the MT, covered by the AMT attributive. The calculation of the indicated operators and the execution of the associated algorithmic procedures are performed according to the samples presented in the procedural patterns.

2) *Procedural patterns* are prescriptions that reflect in symbolic form the content of algorithmic manipulations that should be performed to implement the procedures prescribed by the CM. According to its content the following should be carried out sequentially:

a) calculation of the values of the operators that determine the inductive action of the primary sources and the kernels of the integral equations given by attributes B1 — B3 of the model task;

b) calculation of coefficients and right parts of SLAE, which approximates the IE, to compile the appropriate matrix equation;

c) iterative process of SLAE solution with regularization on each step [11, 12];

d) computing the values of unknown functions of physical fields localization and integrated parameters of numerical layouts of ECT modes according to attributes S1 — S4.

In accordance with the given list of procedures, it is necessary to compose four turns of such patterns, denote them by T1, T2, T3, and T4, respectively.

In general terms, the prescriptions represent a binary predicate form [19] that contains

- indications of the objects of manipulation "O", that is, an abstract name of the categories of objects in relation to which actions determined by the codifier should be performed;
- the manipulation formula "F", that is, an abstract predicate of the procedure, which reveals the content of actions taken relative to the object (use or transformation)
- indicationof the product of manipulation "P", that is, the abstract name of the category of the object obtained as a result of manipulation.

C. The pattern T1 designated to perform operations according to item (*a*) and (*d*) has the form of expression (10):

$$\boldsymbol{W}_{\alpha,\beta} \xrightarrow{\varphi(\beta,\alpha)} \boldsymbol{U}_{\alpha}. \qquad (10)$$

The "O-F-P" components of this pattern are $\boldsymbol{W}_{\alpha,\beta}$, $\varphi(\beta, \alpha)$ and $\boldsymbol{U}_{\alpha}$ respectively. Such a pattern is used to compute the result of the action of sources defined on the set β in the form of the vector $\boldsymbol{U}_{\alpha}$ defined on the set DE of the domain α. A symbol $\boldsymbol{W}_{\alpha,\beta}$ represents any of the structural patterns represented by expressions (9) or other forms related to them. A symbol $\varphi(\beta, \alpha)$ means an operator, by means of which the values of the elements of the vector $\boldsymbol{U}_{\alpha}$ is directly calculated based on data of the pattern $\boldsymbol{W}_{\alpha,\beta}$.

The specific names of the object $\boldsymbol{W}_{\alpha,\beta}$, product $\boldsymbol{U}_{\alpha}$ and type of operator $\varphi(\beta, \alpha)$ of calculating procedure are set by the software module that is selected from the SSSM by attribute codes B1 — B3. The list of these attributes covers those types of operators that may be used in a procedure of the form (10) consistent with attribute A5. The main of them are given in [11] as operators of the basic system of integral equations, but, obviously, it will be appropriate to reproduce them that we will do further.

D. PatternT2 for performing operations according to item b) has a more specific content.

The first step according to this pattern is to calculate the values of the elements of the square matrix of the IE kernel using the patternT1 and calculate the values of the elements of the vector of the right-hand side of the integral equation defined in the domain $\boldsymbol{S}$:

$$\boldsymbol{D}_{i,j} \xrightarrow{\kappa(i,j)} \boldsymbol{Y}_{i,j};$$

$$\boldsymbol{B}_{i,h} \xrightarrow{\tau(i,h)} \boldsymbol{F}_{i}. \qquad (11)$$

Operators $\kappa(i,j)$ and $\tau(i,h)$ in these expressions are included in the list of operators covered by the abstract name $\varphi(\beta, \alpha)$.

The next step in the pattern T2 provides the formation of SLAE relative to the sought function $\boldsymbol{g}_i$ that reflects the density of secondary sources distribution on the boundary surface $\boldsymbol{S}$ of the simulated object (*it is this function that is the key link of CM, which determines all other physical phenomena and processes of ECT*):

$$\boldsymbol{g}_i \in \boldsymbol{G}\big|_S;$$
$$\boldsymbol{Y}_{i,j} \mapsto \boldsymbol{M}_{i,j}\left(\boldsymbol{Y}_{i,j}\right): \boldsymbol{M}_{i,j} = \left[\lambda \cdot \boldsymbol{Y}_{i,j} + \delta \cdot \boldsymbol{I}_{i,j}\right]; \qquad (12)$$
$$\Rightarrow \boldsymbol{M}_{i,j}\boldsymbol{G}_i = \boldsymbol{F}_i.$$

In this expression λ is a scalar coefficient, $\boldsymbol{I}$ is a unit (diagonal) matrix, and δ = 1 for IE of the second kind, or 0 for IE of the first kind.

The matrix equation formed at the end of the chain (12) falls under the standard algorithm of solution by inversion of the SLAE coefficient matrix:

$$\boldsymbol{G}_i = \boldsymbol{M}_{i,j}^{-1}\boldsymbol{F}_i, \qquad (13)$$

but it should be taken into account that through the specific properties of most categories of field sources, the coefficient matrix of the system (12) may be ill-conditioned, and the solution (13) may be incorrect (unreliable) [20]. To eliminate this drawback, one applies the regularization of the IR by modifying its kernel by a calibration term directly in the square brackets of expression (12). However, as the authors of [21] point out and the own experience of the authors of this article testifies, this manipulation does not guarantee a reliable result, so the authors in the developed SCM preferred a more reliable method — an iterative procedure with regularization at each step [10]. So, the following pattern contains instructions for performing such iterative process.

E. PatternT3 is presented in application to IE of the 2nd kind. The usual iteration scheme looks like this:

$$\boldsymbol{G}^{(0)} = 0\,,\ \boldsymbol{G}^{(n+1)} = \boldsymbol{F} - \lambda\cdot\boldsymbol{Y}\boldsymbol{G}^{(n)}, \qquad (14)$$

where n is the number of iteration; $\boldsymbol{G}^{(n)}$ is the vector at current iteration step, $\boldsymbol{G}^{(n+1)}$ is the same at the next step. However, in the algorithm introduced in the SCM, before undertaking every subsequent iteration step, one calculates the average on the set $\boldsymbol{S}$ value of the deviation ε of vector $\boldsymbol{G}^{(n)}$ elements from the calibration constant $\boldsymbol{C}_g$ for a given source type (according to the attribute B1):

$$\varepsilon_g^{(n)} = \left\langle \boldsymbol{g}_i^{(n)} - C_g \right\rangle\Big|_S. \qquad (15)$$

Then this value is applied to the elements of vector $\boldsymbol{G}^{(n)}$ as corrigendum and at the next step already corrected values are used:

$$\boldsymbol{G}^{(n+)} = \left(\boldsymbol{g}_i^{(n+)}\right) = \left(\boldsymbol{g}_i^{(n)} - \varepsilon_g^{(n)}\right) \rightarrow \\ \rightarrow \boldsymbol{G}^{(n+1)} = \boldsymbol{F} - \lambda\cdot\boldsymbol{Y}\boldsymbol{G}^{(n+)}. \qquad (16)$$

Iterations are completed according to the designated criterion of deviation smallness, for example,

$$\varepsilon \le \left\langle \left|\boldsymbol{g}_i^{(n+1)}\right| \right\rangle \cdot 10^{-3}.$$

F.PatternT4 coincides with the patternT1 for calculating the localized parameters of physical fields, but to calculate the integrated characteristics, the geometric basis of this pattern is based on 1D matrices $\boldsymbol{Q, P, Z}$.

Operators of SSSM software modules and their application. Integral operators and some other algorithmic manipulations that are used in procedural patterns (10-16) are specified in attributes B2-B3 and presented in the form of abstract prescriptions. Here is a more detailed description of the main operators. First of all, 3D models of ECT tasks use the operators of scalar φ and vector $\boldsymbol{A}$ of volumetric and surface potentials of a simple and double layer of the form:

$$\varphi_v(P) \triangleq \int_{\Omega_v} g_v(M) K_v(P,M)\, d\omega_M; \\ \boldsymbol{A}_v(P) \triangleq \int_{\Omega_v} \boldsymbol{j}_v(M) K_v(P,M)\, d\omega_M, \qquad (17)$$

where Ωv is the domain of their definition. The type of potential is indicated by the index v that takes a value of 1, 2 or 3 for a simple (1) or double (2) layer or volumetric (3) sources, respectively; g and $\boldsymbol{j}$ are the density distribution of scalar and vector sources; M and P — points of integration and observation.

The kernels of these operators K_v (P, M) have the form:

$$K_1(P,M) = K_3(P,M) = \frac{1}{r_{P,M}}; \\ K_2(P,M) = \frac{\partial}{\partial n_M}\left(\frac{1}{r_{P,M}}\right) = \frac{\cos\psi_M}{r_{P,M}^2}, \qquad (18)$$

where r_{PM} is radius vector from point M to point P; $\cos\psi_M = \cos(\overline{r}_{P,M}, \overline{n}_M)$. These expressions are antiderivative functions for a group of operators, which are determined by derivatives with respect to the coordinates of a point P:

$$K'_{1,\xi_P}(P,M) = K'_{3,\xi_P}(P,M) = \frac{\partial}{\partial \xi_P}\left(\frac{1}{r_{P,M}}\right),$$
$$K'_{2,\xi_P}(P,M) = \frac{\partial}{\partial \xi_P}\frac{\partial}{\partial n_M}\left(\frac{1}{r_{P,M}}\right) = \frac{\partial}{\partial \xi_P}\frac{\cos\psi_M}{r^2_{P,M}}, \quad (19)$$

Where ξ_P is any coordinate of point $P(x, y \text{ or } z)$.

The operators from group (19) are used, in particular, to form the vector derivatives of the kernels (18) $-\text{grad}_P(K_v)$, $\text{rot}_P(K_v)$, $\partial/\partial n_P(K_v)$, and $\text{div}_P(K_v)$, which are necessary for computing the local parameters of the fields distributed in the volume (index $v = 1, 2$ or 3).

Since in ECT tasks 2D approximation is often used, it is worth to cite the basic operators for 2D models as well, where to simplify the notation instead of points indices are given:

$$K_1(i,j) = \ln r_{i,j};\ K_2(i,j) = \frac{\cos\psi_j}{r_{i,j}};$$
$$K'_{1,\xi_i}(i,j) = \frac{\cos\varphi_i}{r_{i,j}};\ K'_{2,\xi_i} = \frac{\cos(\psi_j + \varphi_i)}{r^2_{i,j}}, \quad (20)$$

where φ_i is the angle $(\overline{r}_{i,j}, \overline{n}_i)$.

The outlined method of CMs synthesis in the SCM environment is applicable to a wide range of problems arising at the research of ECT processes, within the scope of one article there is no possibility to describe them in detail, but as an example of its use, we present some results of calculations for the actual statements of MT.

Results of calculations for the selected ECT problems. At the ECT processes, along with the spatial distribution of current density in the ladle volume with melt, the presence and behavior of inclusions — microparticles with other physical and chemical properties — is an essential factor influencing the formation of the casting structure. To investigate this influence, test calculations of the fields and mechanical forces arising from the interaction of induced charges with the excitation field were performed. Below we give some examples of such calculations.

A. MT disposition: in the field created in unlimited space by two electrodes with potentials of opposite signs, there is a microparticle with higher conductivity relative to the medium, for example, a copper particle in a lead melt (the calculations are performed in relative units). To perform the calculation of this MT, the CM is composed. According to *Takstrum*, it is defined by the following codes:

Amodtask = [001, 110, 010, 010, 001, 001];
Bmattool = [010, 010, 001∩011, 001];
Ccalctool = [001, 001, 010, 100].

Fig. 5 shows a map of field equipotentials for this case [11].

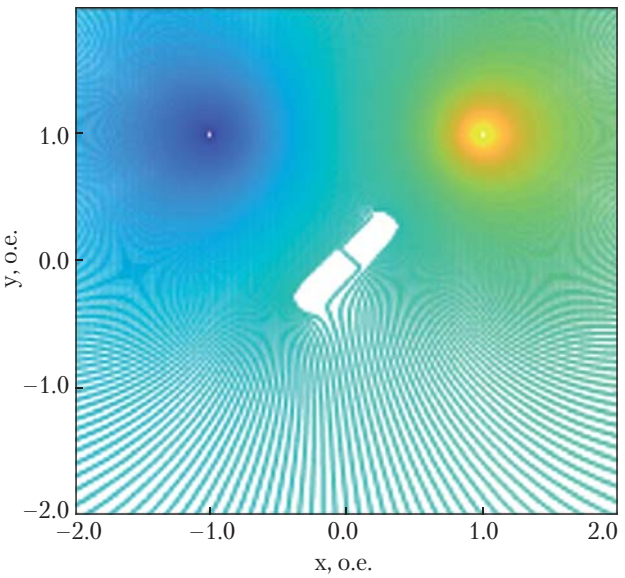


Fig. 5. Map of electric equipotentials of conductive microparticle in the field created by two electrodes

B. MT, derivative (secondary) of the previous one: in the conditions of the MT, shown in Fig. 5, the microparticle is acted upon by forces that arise as a result of the interaction of the primary field with the charges induced on its surface, as they need to be counted. For this, the CM is linked, which is defined by the following codes:

Amodtask = [001, 110, 011, 011, 001, 001];
Bmattool = [010, 010, 001∩011, 010∩011];
Ccalctool = idem.

Figure 6 shows the diagrams of the distribution of surface specific forces vectors acting on a microparticle under the specified conditions [22]. The combination of these forces creates a resul-

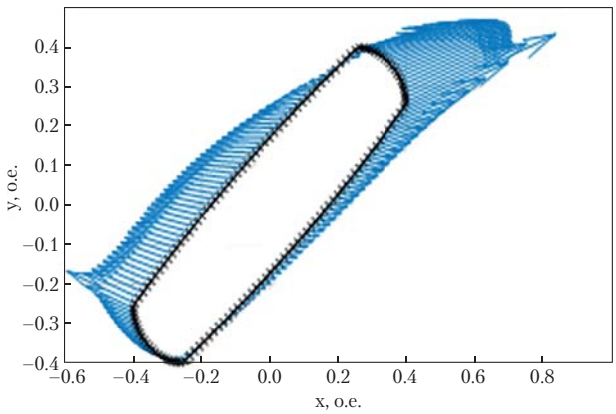


Fig. 6. Distribution of specific surface forces acting on a microparticle in the field shown on the Fig. 5

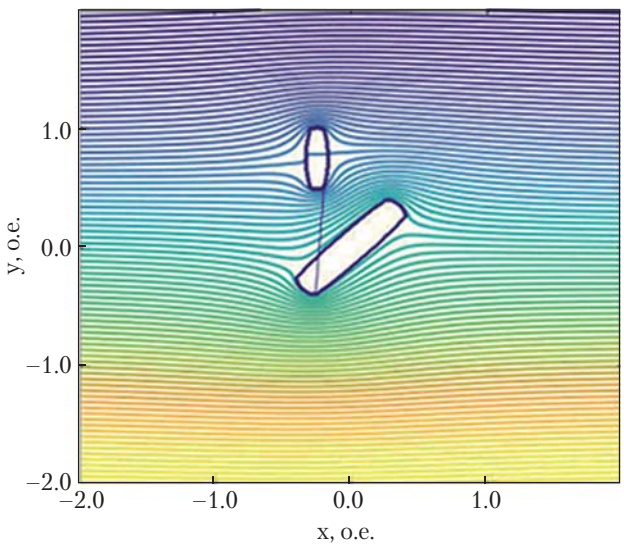
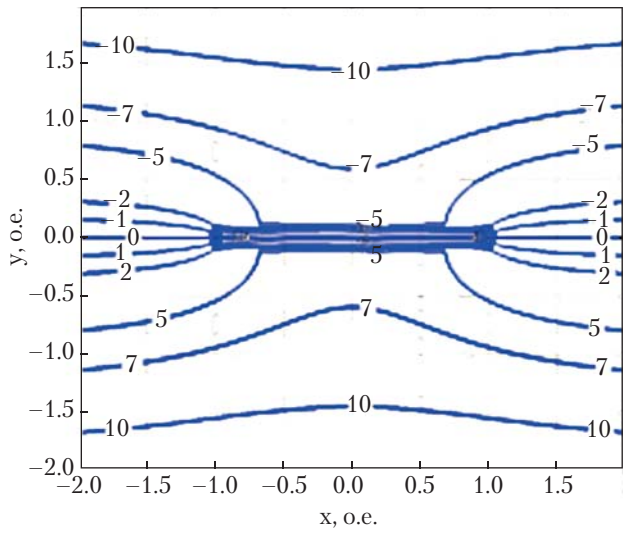
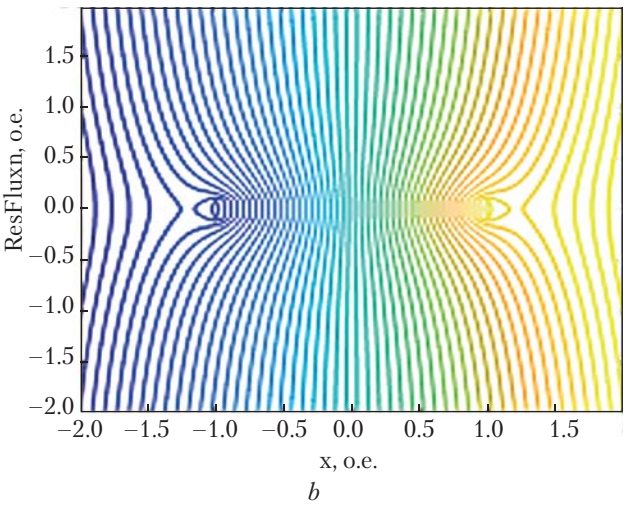


Fig. 7. Equipotentials of two micro-particles in the uniform field



a



b

Fig. 8. Equipotentials (*a*) and flow lines (*b*) of thin sheet (2D-version) in the uniform field

tant force directed at an angle ≈ 60° to the x-axis, which pulls the particle to the "light" electrode, as well as torque that rotates it clockwise.

C. An example of a two-coupled MT, disposition: in a uniform field between flat extended electrodes (like the covers of a capacitor) there are two different particles of an arbitrary shape with high conductivity (similar to the previous MH). The CM is composed by the following coding:

Amodtask = [001, 110, 100, 010, 001, 001];

Bmattool = idem; Ccalctool = idem.

Figure 7 shows the distribution of the field equipotentials for this case [11].

D. MT disposition: the same as the previous one, only instead of two particles, a thin plate is placed across the field (with a ratio of thickness to length of 1: 10). This task is typical for electrostatics where thin sheet electrodes are used in various devices [22]. A feature of this CM is the need to split the integration contour into a large number of small DEs due to the close distance of the opposite sides of the plate, but other studies

will show how to get around this complication. Figure 8, *a* shows the distribution of field equipotentials for this case, and Figure 8, *b* — flow lines.

The given examples of solving some model tasks of ECT by means of integral equations clearly manifest the available possibilities for synthesis of computer models of various problems arising while investigating the processes of melts ECT, by combining different types of algorithmic patterns and specialized software modules that are embedded in the libraries of PPCM and SSSM blocks and coupled with the use of the attributes of *Takstrum* codifier. The number of CMs that can be compiled according to this technique for direct, derivative and related multiphysical tasks, according to preliminary estimates, exceeds one and a half hundred options. This property is a good basis for the introduction of a broad program of in-depth study of the regularities of complex impact of physical fields on the formation of the structure of castings and quality indicators of cast products.

Thus, the proposed SCM provides practical opportunities for full implementation of the concept that was developed by the authors [7] of creating an automated system for controlling the modes of electric current treatment of the melt.

Due to impossibility of direct control of the physical parameters of electric current treatment in the liquid metal medium, the methods of numerical modeling of multiphysical processes of ECT are extremely important for the implementation of controlled effects on the formation of the structure of castings.

The complexity of physical phenomena and the multifactorial nature of their interrelationship in these processes have necessitated the use of unconventional format of mathematical models of ECT problems, which the authors have unified by formalizing the integral equations of heterogeneous multiphysical processes on the basis of their similarity. Such format in terms of methodological unity, physical adequacy and computational efficiency has the certain advantages over conventional ECT models stated via differential equations.

Based on this format of mathematical models, an innovative pattern-module system of computer modeling of ECT processes is developed: methodological foundations for its devising and SCM structure that is represented by a library of functionally related algorithmic modules, the software basis of which is the mathematical apparatus of integral equations, are worked out.

Adequate reflection of the phenomenological content of multiphysical ECT processes in computational algorithms is ensued in the SCM by means of a taxonomic codifier created by the authors, which gives an opportunity to codify in binary code a considerable number of individual tasks characteristic of multiphysical ECT processes on a combinatorial basis.

Due to this, the flexibility of the pattern-module architecture of computer modeling algorithms in terms of its adaptation to a wide range of multiphysics processes is achieved. At the same time for concise display of algorithmic procedures a new formalized symbolic-matrix notation of prescriptions to perform the corresponding computational operations was introduced.

Approbation of SCM application to the tasks of modeling the electric field and forces of interaction of induced (secondary) sources with the primary field under different conditions of simulation of melt ESO processes proved its complete operability.

The prospect of further practical application and development of SCM architecture consists in detailed elaboration of algorithms for calculating quantitative estimates of energy impacts and synthesis of numerical layouts of ECT modes and full implementation of the authors' concept of automated control system of melt electrochemical treatment modes to improve the quality of castings and production processes efficiency.

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ІННОВАЦІЙНА СИСТЕМА КОМП'ЮТЕРНОГО МОДЕЛЮВАННЯ МУЛЬТИФІЗИЧНИХ ПРОЦЕСІВ КЕРОВАНОЇ ЕЛЕКТРОСТРУМОВОЇ ОБРОБКИ РОЗПЛАВУ

Вступ. Широке застосування литих виробів з алюмінію та його сплавів потребує забезпечення якісної структури виливків, від якої залежать їхні експлуатаційні властивості. Керувати процесом формування якісної структури виливків можливо, зокрема, методом електрострумової обробки розплаву.

Проблематика. Через недоступність розплаву для прямого вимірювання параметрів процесу обробки єдиною можливістю реалізувати керування режимами обробки є їх чисельне моделювання. Але складність та взаємозалежність мультифізичних процесів електрострумової обробки розплаву обумовила нетрадиційний підхід до формулювання їхніх математичних моделей та обчислювальних процедур, що визначило особливості завдань щодо побудови відповідних комп'ютерних моделей та їх застосування.

Мета. Розробка новітньої шаблонно-модульної системи комп'ютерного моделювання мультифізичних процесів електрострумової обробки розплавів для керування режимами формування якісної структури виливків.

Матеріали та методи. Матеріалом дослідження є сукупність модельних задач мультифізичних процесів електрострумової обробки, їх онтологія, інтегральні рівняння цих процесів та їхні властивості, а також бази даних про параметри модельованих об'єктів. Використано метод онтологічної таксономії, здійснено систематизацію модельних задач і математичних інструментів їх розв'язання, застосовано метод формалізації інтегральних рівнянь пов'язаних мультифізичних процесів.

Результати. Розроблено уніфіковані шаблони основних алгоритмічних процедур та бібліотеку програмних модулів обчислювальних операцій часткових задач, кожній з яких присвоєно унікальний код згідно з кодифікатором. Комбінування шаблонів з різними модулями, які ідентифікуються за вказаними кодами, забезпечило можливість формувати широкий спектр комп'ютерних моделей процесів обробки. Побудовано гнучку систему комп'ютерного моделювання мультифізичних процесів і підтверджено її працездатність при симуляції режимів електрострумової обробки розплавів.

Висновки. Отримані результати забезпечують можливість керування режимами електрострумової обробки розплавів для формування якісної структури литого металу.

Ключові слова: електрострумова обробка, розплав, мультифізичні процеси, таксономічний кодифікатор, математичні моделі, комп'ютерне моделювання, шаблон, модуль.