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INTELLIGENT DECISION SUPPORT SYSTEM

Gennady Shvachych, *Doctor of Science, National Metallurgical Academy of Ukraine, Dnipro, Ukraine, ORCID ID: https://orcid.org/0000-0002-9439-5511*
Ivan Pobochij, *Doctor of Science, National Metallurgical Academy of Ukraine, Dnipro, Ukraine, ORCID ID: https://orcid.org/0000-0001-7023-1857*
Maryna Sazonova, *Candidate of Science, National Metallurgical Academy of Ukraine, Dnipro, Ukraine, ORCID ID: https://orcid.org/0000-0002-9513-9659*
Oleksandr Bilyi, *Candidate of Science, National Metallurgical Academy of Ukraine, Dnipro, Ukraine, ORCID ID: https://orcid.org/0000-0003-1234-5404*
Dmytro Moroz, *Master, Oles Honchar Dnipro National University, Dnipro, Ukraine, ORCID ID: https://orcid.org/0000-0003-2577-3352*

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information system, data analysis, information storages, intelligent decision.

ABSTRACT

Here one of the new efficient approaches to solving problems of intelligent support of making decisions of a cooperate enterprise scale is analyzed, bearing in mind that the enterprise is oriented towards integration of two interconnected information technologies: a technology of constructing information storages and a technology of intelligent data analysis.
A new conception of the role of informating-controlling systems in controlling and operating pipe manufacturing process is suggested. It broadens a traditional view over information systems just as if it were only an instrument of a computer data analysis. The role of the modern information systems in the manufacturing as an independent scientific and applied direction serving as a connecting link in the triad "raw product – ngineering process – end product" is substantiated. Some problems connected with plantation of the informating-controlling systems in the pipe manufacturing is formulated. It broadens a traditional view over information systems just as if it were only an instrument of a computer data analysis. The practical application of this product permits the operating personnel of the enterprise to control the engineering process, analyze the processes passing in each mill, adjust the PRP mills' engineering characteristics in the pipe-manufacturing process. The suggested approach influences quite strongly the production's quality improving and enables to work stably in the thin-walled pipe grades sphere.

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Introduction. Nowadays, the informating-controlling systems alongside with expert-logical systems are considered essential instruments of the theory and practice of manufacturing. At the same time, the sphere of the informating-controlling systems is very deep, varied and wide, it requires knowledge and an active using of the results of different sections of computer-information preparation, mathematics, system analysis, statistics, engineering process of manufacturing. In fact, nowadays, this sphere pertains to the fundamental basis of technological research of the product and of efficiency of the manufacturing in whole.

During all the development period of the direction and especially in the recent years, its extreme importance for the product's quality improving and working efficiency increasing has been pointed out. That is why, as the informating-controlling systems were developing, they were getting associated in a single system of the engineering process and manufacturing control.

A lot of works are devoted to the problem of research, elaboration and plantation of the computer systems in metallurgy. So, in [1] the role of the computer control systems in cast iron production is accentuated. In [2] it is shown that the computer control systems allow to realize not only a current fusion control, but also to conduct an analysis of the technological situations with giving recommendations as to controlling the blast-furnace process in whole. In [3] it is noted that the software environment for conducting a calculating analysis of the most important sides of the blast-furnace process and for conducting an automated search for the optimal conditions of fusion in basic modes of the blast furnace's performance

In [4] a new approach to mathematical modeling of metal turning in section extruding based on the finite elements method is suggested.

In this article, one of the efficient approaches to solving problems of intelligent support of making decisions of a cooperate enterprise scale is analyzed, bearing in mind, that the enterprise is oriented towards integration of two interconnected information technologies: the technology of constructing information storages and the technology of intelligent data analysis. Additionally, in our opinion, the information systems, correspondent mathematical models and processes of their construction, verification and interpretation are the irreplaceable link in the triad "raw product – engineering process – end product", and they are called to provide integrity of the engineering process and manufacturing. Besides, prospects of a further development of informating-controlling systems, both in pipe manufacturing and in some related researches supporting this direction are examined.

Setting the problem. Upgrading of technics and technologies and a continuos growth of requirements to the quality of the product inspire elaboration of new information systems of intelligent support of making decisions of a cooperative enterprise scale.

One of the approaches to creating systems of a new generation decision support is oriented towards integration of two interconnected information technologies: the technology of constructing information storages (IS) and the technology of intelligent data analysis.

This article is devoted to the peculiarities of elaboration of the information systems of the new type on the example of the controlling processing characteristics of the products rolled by the pipe-rolling plant 140 (PRP-140).

Nowadays, the technology of constructing IS is partially based on the PRP-140 with lengthwise-rolling mills. Let us have a look at the process of its construction (fig. 1).

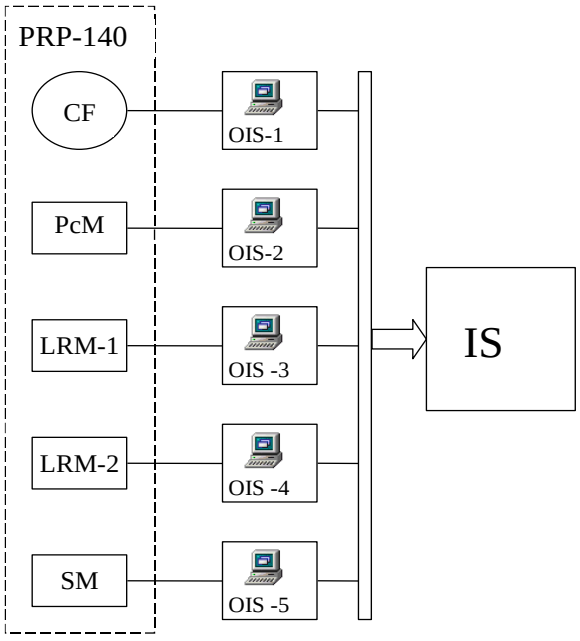

Fig. 1. Structural scheme of the information system

In the fig. 1, we use the following abbreviations: CF – circular furnace; PcM-piercing mill; LRM-1 and LRM-2 – lengthwise rolling mills No1 and No2; SM – sizing mill; OIS-1, OIS-2, OIS-3, OIS-4 – operative information systems, IS – information storage.

The substance of the constructing technology of the IS is as follows. The distinctive feature of the engineering process of the pipe manufacturing by the PRP-140 with the lengthwise-rolling mills is in presence of single-type structural elements in the plant line which define the composition and configuration of the PRP-140. Such a peculiarity allows to create the OIS which contains a varied information as to the performance of the PRP-140 (date, time, fusion number, pipe grades, steel quality etc.). Further on, the data from the OIS are extracted and put into one source – the IS.

The main idea, put into the principle of the IS technology is to conduct the current analysis intermediately on the basis of the operative information systems is inefficient. It is explained by the fact that the data as to the performance of one of the PRP-140 mills do not enable to get a whole and objective picture of the performance of the plant in whole. All the necessary for the analysis data are kept in a single source – the IS. The main peculiarity of the IS data is their availability not only for reading. At the same time, no data modification is made, as it may break integrity of the IS.

It should be noticed that the IS, according to their classical definition, are a set of facilities permitting to give integral data for their further analysis and making decisions as to the control. It means that the information storages give only a long-range architecture of the intelligent cooperative enterprise scale decision system construction, and they are its central part. The task of the research suggested is to elaborate a set of special software environment, which would enable to construct a polyfunctional system of intelligent decision-making, where such software environment is oriented towards the analytical data processing technologies – the technologies of intelligent data analysis (IDA). Then the above-mentioned technologies must be integrated for making correspondent decisions as to adjusting the processing characteristics of the rolling process.

Software environment system. In order to solve the tasks set, a software environment system was elaborated. It requires the following resources:

– Operating system: Microsoft Windows−95 and higher or Microsoft Windows NT 4.0 and higher.

– On-line storage: 16 Mb (32Mb is recommended). For Windows NT 4.0 48 Mb is recommended.

– Internet Explorer 3.0 (or of more modern versions).

– MS Office 97 or higher composed of Database Management System Access, MS Excel.

– MathCad of 2000 Version or higher for data processing.

– During installation of the software environment a setup box appears, wherein one can indicate the correspondent modes. At this stage, it is possible to refuse some modes. Other settings may be used later.

Information system of intelligent support of decision-making. You can see the structural scheme of the information system of intelligent support of decision-making in the fig. 2. Here, ISISD stands for the information system of intelligent support of decision-making.

Taking into consideration that the IS contain various information as to the performance of the PRP-140 (date, time, fusion number, pipe grades, steel quality, ingoing size of the round billet, pipe sizes after each mill etc.), the task of the suggested information system is to classify and to process the data for the purpose of resetting the PRP-140 mills' processing characteristics and those of the correspondent forecast.

At the same time, the information system enables to take a lot of measures as to the data processing. So, if necessary, one can follow dynamics of changing the characteristics of each pipe from the circular furnace up to the sizing or reducing mills inclusively. Besides, there appears a possibility to classify the data according to the rolling characteristics (steel quality, ingoing size, round billet size, pipe grades etc.). The latter permits to carry out a number of researches connected with determining dependence of the rolling process results on the ingoing data and current characteristics.

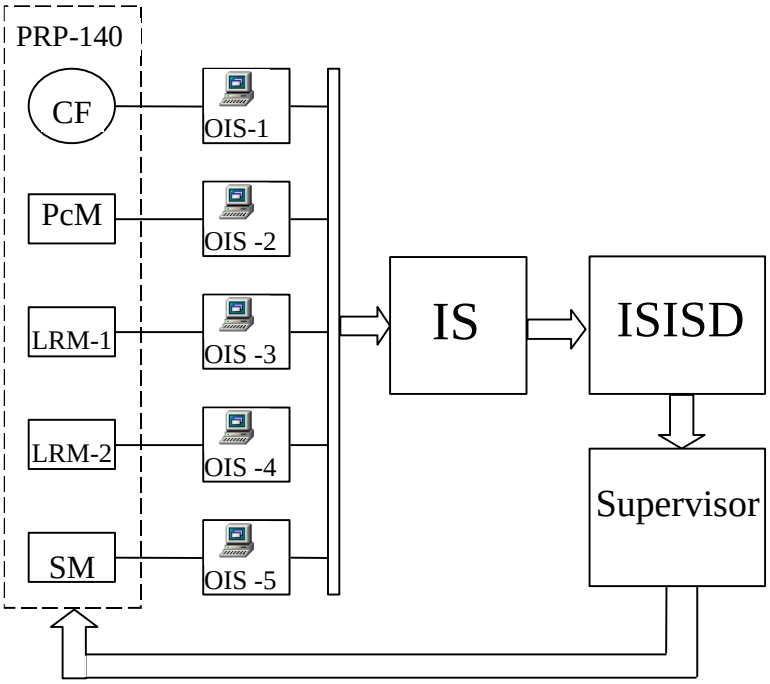

Fig. 2. Structural scheme of the information system of intelligent support of decision-making

For example, in the process of piercing a lot of one-sized hollow-billets, an elongation ratio shift under each hollow billet's deformation may be observed [5]. A variable pace of work of the piercing mill, preconditioned by essential processing pauses, implies a constant considering of the thermal condition of the plant which influences the total elongation value. The elongation ratio shifts under a lot of hollow billets piercing reach 30% of nominal (table) values. In order to stabilize the elongation ratio, the operating personnel (supervisor), following his own practical experience and intuition adjusts the mill settings by means of shifting the piercer plug before piercing the next hollow billet. For the purpose of reducing the supervisor's subjective influence, the suggested system chooses the required piercer plug's condition subject to the algorithm elaborated.

The suggested system is oriented towards application of the method of the exponential average magnitude, as a method which describes the process of the elongation ratio shifting process μ_{pr} of the piercing mill in the most accurate way. It is presented as a time series, and the exponential smoothing of the elongation ratios series is calculated according to the recurrent formula:

$$\mu_{pri} = \alpha \cdot x_i + \beta \cdot \mu_{pri-1},$$

where μ_{pri} is the exponential average magnitude (elongation ratio) at the point of time t_{pr};

α is the smoothing characteristics; $\alpha = const$, $0 < \alpha < 1$, $\beta = 1 - \alpha$;

μ_{pri-1} is the real elongation ratio under piercing the next hollow billet;

x_i is the time series.

The software support of the information system (IS) is constructed according to the algorithm which, in the final analysis, allows to receive the current pipe characteristics shifts from those given, or from those weighted average; and also the dependencies of the shifts upon the rolling processing characteristics. So, in order to examine the metal crop volume it is necessary to estimate the rolled pipes' length's $l_{\phi i}$ deviations from the nominal (table) pipe length value (l_{Ti}): $\Delta l = l_{\phi i} - l_{Ti.}$ Estimation of the length deviations volumes is made by comparing the actual lengthes with their average magnitude (l_{av}) for the lot:

$$\Delta l = l_{\phi} - l_{av},$$

where $\Delta l = \frac{1}{n}\sum_{i=1}^{n} l_{\phi_i}$,

where n is the number of the pipes rolled.

In order to estimate the received rolling characteristics, the algorithm uses the dependencies including the peculiarities of the pipe deformation process according to the fundamentals of the pipe manufacturing theory [6]. It should be noticed that among the analyzed characteristics, the principal figures are those of the hollow billets' and pipes' length, the elongation ratios for each mill and the plant in whole, crop values, dead time, unfinished sections number. Let us consider a variant of the suggested IS's functioning.

Example of the is's functioning. The suggested IS provides for several functioning modes. A large volume of information in the IS requires a preliminary data retrieval, which is made by means of classifying according to the date, pipe grades, fusion number, lot's number, order's number. Let us consider an example connected with the data processing and analyzing according to the calendar.

When switch to the calendar mode, a dialog box appears on the screen for the user to choose the year, month and day, for instance, as it is shown in the fig. 3. The user has decided to analyze the information for the 24 working hours of 21 March, 2021 of the PRP-140.

Fig. 3. IS calendar's working mode

Subject to the chosen date the IS data retrieval is activated. In the result of processing the information, the total number of records on this issue appears on the screen (fig. 4).

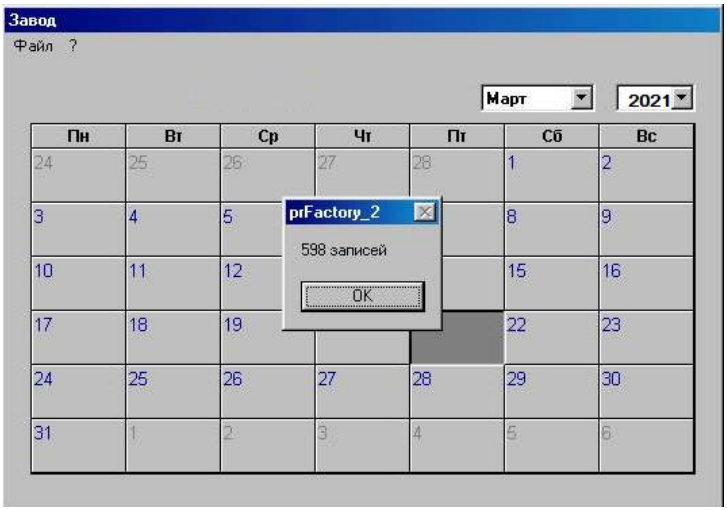

Fig. 4. IS data's analysis subject to the chosen date

Further on, the information as to the functioning of the PRP that day in whole appears on the screen. (fig. 5).

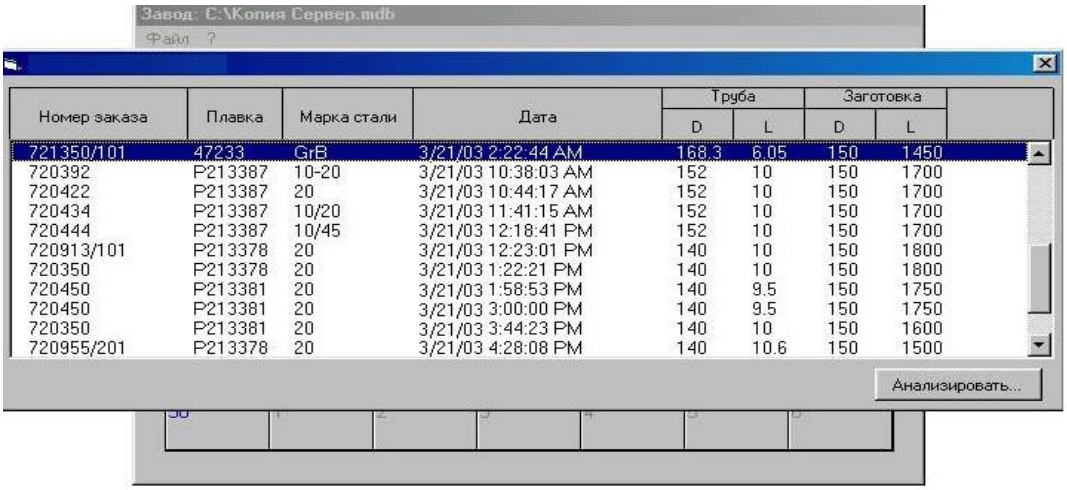

Fig. 5. Data as to the PRP's functioning for 21/03/21

In this box, numbers of orders for pipe manufacturing, hollow billets sizes, the rolled pipes grades, rolling time etc. are shown.

If necessary, the required information can be printed out and analyzed (press the button "Analyze"). Here the data from the IS are transferred to the Excel environment, where their automatic classification and processing according to the algorithm is given.

The data transfer from the IS to the Excel environment is explained by the fact that the given program product enables to realize the necessary data processing in rather a convenient and obvious manner. In the fig. 6, a fragment of processing the data as to the piercing mill and lengthwise-rolling mills No1 and No2 with the given length of the hollow billet before piercing and after heating is shown.

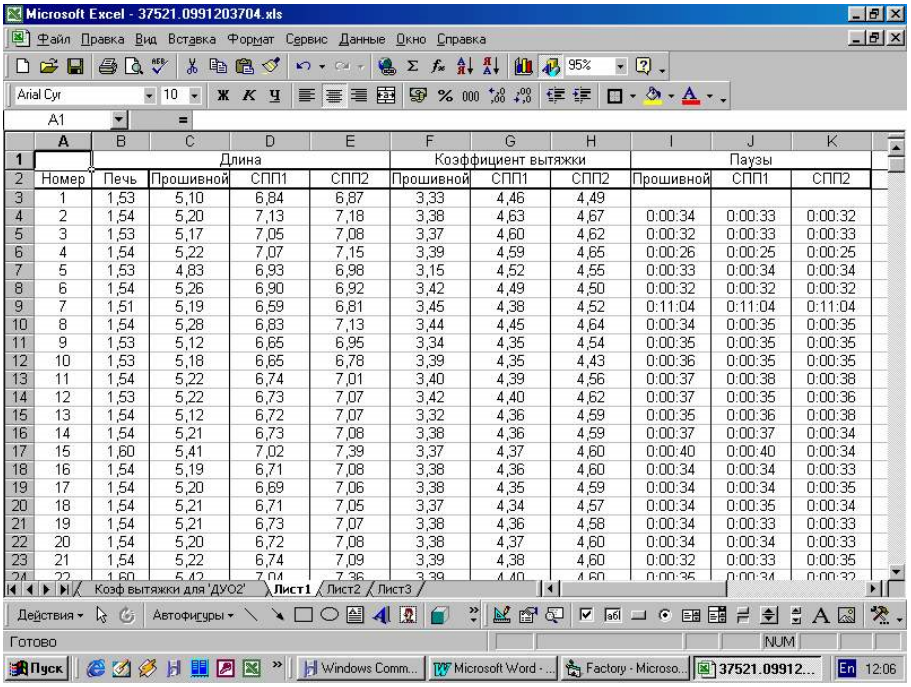

Fig. 6. Data analysis in the Excel environment

Besides the analytical procedure of information processing, the environment permits to form the required graphical dependencies (drawing 7).

As an example, let us examine a process of rolling a pipe of 168 mm diameter, 7.00 mm wall thickness and 6,000 mm length. In the table (fig. 6) the data as to the pipes' length, elongation ratios and processing pauses for the plant's mill are presented. The calculation (table) values of the following processing characteristics: the summary elongation ratio is 4.9; the elongation ratio on the piercing mill is 3.41; in the LRM-1 – 4.40; in the LRM-2 – 4.56.

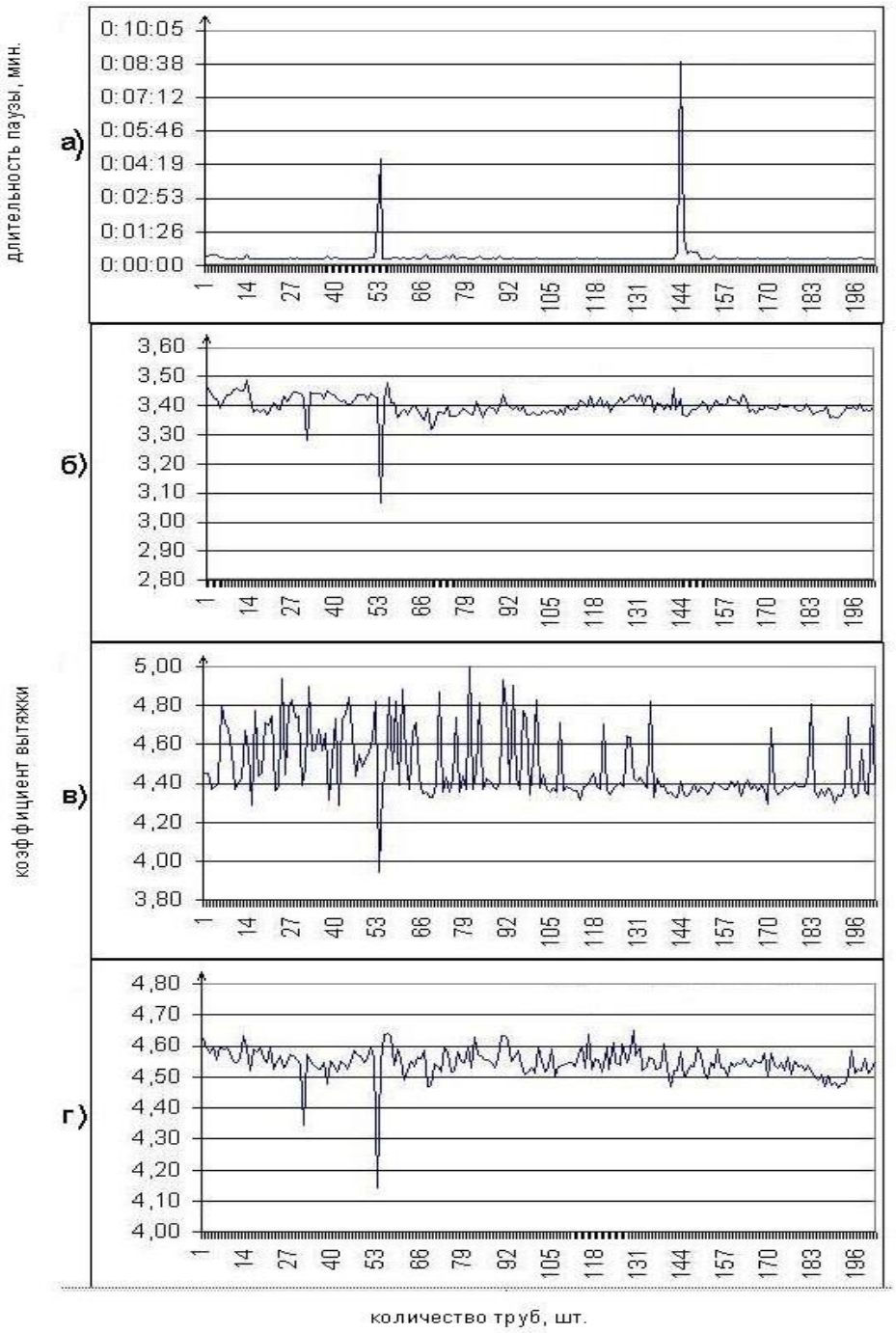

Fig. 7. Elongation ratio changes and the pipe sized 168 x 7.0 rolling process porosity; a) – pause duration before the hollow billet piercing; b); c); d) – elongation ratios in the PcM, LRM-1, LRM-2 (per pipes' number (in pieces)).

The pause of 4.5 minutes before piercing the 53-th hollow billet (drawing 1a) led to reducing the elongation ratio on the piercing mill up to 3.08 (drawing 7b) and is observed on the following mills (drawing 7c, d) –in the LRM-1 the elongation ratio reduced to 3.95, in the LRM-2 – to 4.13. It is likely to lead to increasing the No53 pipe's wall thickness, and if the engineering process was passing without the supervisor's intermediation (as confirmed by the data in the drawing 7 c, d), the wall thickness will exceed the limits, so the pipe will be rejected.

Using this information in the on-line mode, the LRM supervisor has a possibility to adjust the mill's settings in order to change the elongation ratio of the LRM-2 up to the value close to that from the table.

Besides the mentioned table and graphical rolling process analysis, the IS enables to give short-term forecasts in the automatic mode with giving recommendations as to on-line adjustment of the mill's characteristics.

Techniques of analyzing the data by the supervisor. When analyze the information, people often come across to the fact that the theoretical excellence of methods of analysis break down against the reality. It is explained by the fact that perfect, from the theoretical point of view, methods of analysis have very little in common with practice. More often, the supervisor faces the situation, when it is rather difficult to do some assumptions concerning the task investigated. It is not always possible to construct a PRP model, and the table of experiment-based data of an "input-output" type, where each line contains values of the input characteristics of the object and the correspondent values of the output characteristics, becomes the only source of information for the rolling process. In the result, the supervisor has to use heuristic or expert assumptions as to the processes developing in the PRP systems. These supervisor's assumptions are based on his experience, intuition, depth of understanding of the analyzed engineering process. The conclusions drawn from such an approach are based on a simple but fundamental hypotheses about monotony of the decision space. This hypotheses may be expressed as follows: "Similar input situations lead to the similar output reactions of the system". In the result of such a decision-making method, an academic severity is sacrificed to the real situation.

Of course, the supervisor is ready for the analyzed process to turn out to be too sophisticated and not capable of being strictly analyzed with the help of exact analytical methods. Nevertheless, taking into account the information received by means of the ISISD, one can get a pretty clear idea of the PRP's performance in different circumstances, approaching the task from different points of view and following the correspondent data domain. Here, on basis of the ISISD, the process of progressing from a raw model to more adequate ideas of the analyzed process is realized. The flow-block of methods of analyzing the data by the supervisor is presented in the fig. 9.

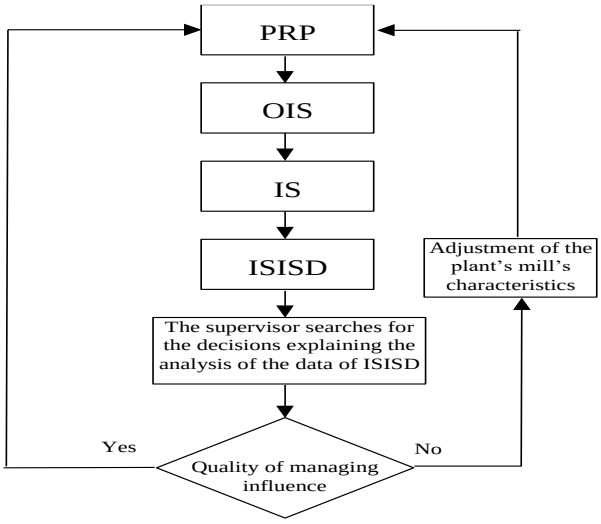

Fig. 9. Flow-block of methods of analyzing the data by the supervisor

The data as to the functioning of various PRP mills come to the OIS which contain information concerning the engineering characteristics of the rolling process. The data are extracted from the OIS and put into a single information source – the IS. The block of data is the basic information for the ISISD. The ISISD enables to process the data as required and to present the data analysis in a suitable table and graphical form. Besides, the ISISD prognosticates adjustment of the plant's mills' characteristics. Following the received information, the supervisor makes the appropriate decision as to the PRP's functioning modes. Here, either an appropriate adjustment of the mills' characteristics is realized, or the rolling process followed by accumulation of information goes on.

Summary. In the suggested approach, the key role in making decisions as to the control belongs to two technologies: the technology of IS and the technology of the intelligent data analysis. The suggested technologies are an essential component of the engineering process and serve as the connecting link in the triad "raw product – engineering process – end product".

The practical application of this product permits the operating personnel of the enterprise to control the engineering process, analyze the processes passing in each mill, adjust the PRP mills' engineering characteristics in the pipe-manufacturing process. The suggested approach influences quite strongly the production's quality improving and enables to work stably in the thin-walled pipe grades sphere.

The principal approach to task-solving may be used for other rolling mills, such as continuous rolling mils, flatting mills, small-section mills, hot-rolling mills that will help to save the metal and improve the quality of production.

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JUMPING FROG METHOD FOR OPTIMAL CLASSIFICATIONS

Kozin I. V.,
Doctor of Physical and Mathematical Sciences, Professor, Zaporizhzhia National University, Ukraine
Selyutin E. K.,
postgraduate student, Zaporizhzhia National University, Ukraine
Polyuga S. I.,
Ph.D., Zaporizhzhia Regional Institute of Postgraduate Pedagogical Education, Ukraine

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ABSTRACT

In the article the problem of finding optimal classifications on a finite set is investigated. It is shown that the problem of finding an optimal classification is generated by a tolerance relation on a finite set. It is also reduced to an optimization problem on a set of permutations. It is proposed a modification of the mixed jumping frogs to find suboptimal solutions of the problem of classification.

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Introduction. Classification is a powerful scientific method. The classification problem arises in almost all areas of knowledge when analyzing research results, when designing and forecasting, when assessing and making decisions. Often having a simple formulation, the classification problem turns out to be quite complex and ambiguous. Moreover, sometimes when trying to classify, interesting paradoxes arise associated with the unification of fundamentally different objects into one class.

The solution to the classification problem, as a rule, includes a significant proportion of subjectivity, individual assessments, fuzzy, informal conclusions. Often the priorities of the decision maker (DM) influence the solution of this problem. This leads to the construction of fundamentally different classifications based on the same primary information. Especially often this situation arises in those areas of knowledge in which it is impossible to use numerical estimates in the classification of objects and phenomena, due to which there is a need for fuzzy assessments, the use of the concepts “similar”.

Formulation of the problem. The aim of this work is to construct metaheuristics for finding a suboptimal classification defined by a tolerance relation on a finite set. This approach allows one to construct partitions close to optimal sets in accordance with the relation of “proximity” of elements. Moreover, this relationship of proximity is not transitive. The proposed algorithms can find wide application in applied problems related to the problem of object classification by a number of attributes. Such problems often arise in the economic, social and technical sciences.

Solution method and analysis of the results. From the point of view of mathematics, the classification problem can be considered from different positions. The main one is the set-theoretic approach when constructing a classification. However, in practice, it turns out that this approach is good only post factum, that is, for clarifying and formally describing an already constructed classification.

The most widespread up to now are statistical classification models, which allow grouping objects according to the results of statistical data analysis [1, 2, 3]. Metric algorithms use the formalization of the concept of similarity between objects and the hypothesis of compactness [2, 3, 4]. There is another principle: the so-called logical classification algorithms. This approach is based on the principle of inductive inference of logical laws or induction of rules [5, 6, 7]. Classification models are becoming more widespread is they are based on the tools of the fuzzy sets theory. A comparatively new direction is classification models based on integral mathematics. An interesting direction is the use of artificial intelligence methods for solving classification problems. An overview of existing recognition methods is given in the monograph [6].

Statement of the classification problem on a finite set

By a partition of a finite set *X* we mean a set of its nonempty subsets $X_1, X_2, ..., X_n$ such that:

1) $\bigcup_{i=1}^{n} X_i = X$;

2) $\forall i, j,\ i \neq j \quad X_i \cap X_j = \varnothing, \quad i, j = 1, 2, ..., n$.

The classification problem on a finite set consists in finding a partition that has some given properties. A set partition defines the canonical equivalence relation associated with this partition. Namely: two elements are considered equivalent if they belong to the same split element. On the other hand, it is easy to show that any equivalence relation on a finite set determines its partition into classes of elements equivalent to each other.

Recall that an equivalence relation on a set *X* is a binary relation " ~ " with the following properties:

1) reflexivity: $\forall x \in X \quad x \sim x$;

2) symmetrically $\forall x, y \in X \quad x \sim y \Rightarrow y \sim x$;

3) transitive: $\forall x, y, z \in X \quad x \sim y, y \sim z \Rightarrow x \sim z$.

Let us present a simple algorithm [8], which allows for a given equivalence relation to construct the corresponding partition of the set *X* into classes of equivalent elements.

Step 0. An arbitrary ordering (numbering) of elements of the set *X*: is chosen $x_1, x_2, ..., x_N \in X$. Here is $N = | X |$. A set of representatives of equivalence classes is determined, which is empty at the initial stage of the algorithm. The set of equivalence classes is also empty.

….

Step *i*. The next element *x of the* ordered sequence of elements of the set *X* is selected and sequentially compared with the set of representatives of already defined equivalence classes. If this element is equivalent to a representative of the class X_k, then it is placed in the class X_k. If it is not equivalent to any of the elements of the set of representatives of the classes, then the element is entered into the set of representatives and defines a new class of equivalence.

The algorithm ends when all elements have been viewed and categorized. The result of the algorithm is a set of representatives of different classes and a set of classes of equivalent elements.

It follows from the transitivity of the equivalence relation that the set of classes obtained as a result of the operation of the algorithm does not depend on the initial ordering of the elements of the set *X* (Step 0). Another ordering can only change the sequence of equivalence classes and the set of representatives. The above algorithm for finding equivalence classes and a set of representatives will be called linear.

Let us note one feature of the linear algorithm. It can be applied not only to an equivalence relation, but also to any binary relation. However, if the relation is not transitive, then the result of the algorithm will already significantly depend on the choice of the initial ordering of the elements.

The relation of tolerance and classification based on the concept of proximity of elements.

Most of the existing classifications in applied sciences are not built on the basis of the equivalence relation, but on the basis of another binary relation - the tolerance relation. Tolerance relation is a reflexive and symmetric relation "$\approx$" on the set *X*, that is, a relation that is determined by the following properties:

1. $\forall x \in X \quad x \approx x$;
2. $\forall x, y \in X \quad x \approx y \Rightarrow y \approx x$.

A typical example of such a relationship is the relation of approximate equality on a set of numbers. In practice, the attitude of tolerance appears in the form of a relationship between objects, which is described by the words “similar”, “close”.

If the tolerance relation “$\approx$” is defined on a finite set *X*, then we can apply a linear algorithm for class allocation and obtain a classification on this set. However, in contrast to the classifications that are based on equivalence relations, classification, constructed on the basis of tolerance relationship, depends essentially on the choice of the initial ordering of the elements of *X*. Different ways of ordering elements can lead to fundamentally different classifications.

Optimality criterion for classifications.

There are many approaches to determining the optimal classification. Informally, a classification is optimal if the elements within the classes are “close enough” to each other, and the classes themselves are “far enough” from each other. Let's consider one of these approaches.

A closeness measure on a finite set X *is a* function $p: X \times X \to R_+$ with the following properties:

1) $\forall x, y \in X \quad p(x, y) \geq 0$ moreover $p(x, y) = 0 \Leftrightarrow x = y$;

2) $\forall x, y \in X \quad p(x, y) = p(y, x)$.

In particular, the distance between points in metric space can serve as a measure of proximity.

Let a positive number be given $\varepsilon > 0$. We will say that the elements $x, y \in X$ are in proximity (close to each other), if $p(x, y) \leq \varepsilon$. This ratio is the ratio of tolerance and, as mentioned above, gives rise to many different classifications, which are defined by the selected ordering on the set *X*. We will call such classifications -classifications. The linear partitioning algorithm changes slightly. Namely: at step *i* there is a class (among the constructed ones), the representative of which is closest to the analyzed element. If the measure of proximity between this representative and the element in question is less than or equal to the value, then the element is added to the class. Otherwise, the element in question becomes a representative of the new class.

The distance between two non-empty disjoint subsets is $A, B \subseteq X$ defined as a function $p(A, B) = \min_{x \in A, y \in B} p(x, y)$.

Let a linear order "$\prec$" of elements on the set X be given, determined by some permutation $s \in S_n$. Let us denote the equivalence classes $X_1, X_2, ..., X_n$ for the ε-classification generated by this order. As a criterion for optimality of classification, we will choose a function $F(s) = \min_{i, j, i \neq j} p(X_i, X_j)$. Then the condition for the optimality of the ε-classification will be the condition

$$F(s) \xrightarrow[s \in S_n]{} \max$$

Such a task is computationally complex [9]. However, the algorithm itself for finding a partition by a given order relation has a polynomial complexity.

Thus, the optimal classification of the search problem is reduced to the problem of finding *an optimal permutation* of the elements of *the X*. This allows us to propose a number of metaheuristics for finding suboptimal solutions to the classification problem [10]. Consider two such metaheuristics, the effectiveness of which has been confirmed by a large number of applications.

Permutation evolutionary algorithm.

The standard scheme of the evolutionary permutation algorithm is used. Let us briefly describe the principle of operation of such an algorithm [10]. The set of all permutations of *n* elements is chosen as the base set of solutions S_n. At the initial step, a set of solutions is constructed using the initial population operator $Y_0 \subseteq S_n$. At each next step, it is assumed that a certain set of permutations is given the current population. At the first step, this is a set $Y = Y_0$. For each of the elements of the set *Y*, the value of the selection criterion is calculated, which in this case is a covering mapping of the original problem. Then, using the selection operator in the current population *Y*, a set of pairs $U = (u_1, u_2, ..., u_n)$ and

$V = (v_1, v_2, ..., v_n)$ is selected for crossover operation. A crossover operator $Cross(U, V)$ is applied to each pair, and then a mutation operator is applied to the result. Permutation – descendant is constructed as follows: sequences *U* and *V are* scanned from the beginning. At the *k* -th step, the smallest of the first elements of the sequences is selected and added to the new permutation – descendant. This element is then removed from the two parent sequences. For instance,

Cross((2,4,7,6,1,3,5,8),(3,8,1,5,4,2,6,7)) = (2,3,4,7,6,1,3,5,8).

The mutation operator *M* performs a random transposition (replacement of two elements) in a permutation with a given probability $\alpha \in (0,1)$.

In this way many elements are found the descendants of $\tilde{Y}$. The evolution operator is applied to the intermediate population $Y \cup \tilde{Y}$, which is the union of the current population and a set of descendants, which selects a new current population on this set. The evolution process is repeated until the condition for stopping the evolutionary algorithm is satisfied. The solution of the original problem is restored from the found permutation.

Mixed jumping frogs method.

The algorithm of the method of mixed jumping frogs is simple to understand and implement, has a small number of parameters, and has been successfully used to solve combinatorial and continuous optimization problems [5,6].

The essence of the jumping frog algorithm for finding the optimal permutation is reduced to the following sequence of steps.

Step 1. Initialize the initial frog population as a set of points in the permutation space with Kendall's metric S_n.

Step 2. Calculate the value of the optimality criterion for each permutation from the initial population.

Step 3. Arrange the solutions in descending order of the optimality criterion value.

Step 4. Divide virtual frogs (solutions) into memplex blocks in such a way that the first virtual frog in the sorted list falls into the first memplex, the second is entered into the second memplex, etc.

Step 5. Find the best s_{k1} and worst s_{k2} solution in each memplex $k \in \{1, 2, ..., K\}$.

Step 6. Try to improve the position of the worst virtual frog by randomly moving it in the direction of the best frog $s = Cross(s_{k2}, s_{k1})$.

Step 7. If the previous operation does not improve the solution, then try to improve the position of the worst virtual frog by moving it towards the globally better frog $s = Cross(s_{k2}, s_{11})$.

Step 8. If the last operation does not improve the position of the virtual frog, then instead of it, randomly create a new frog in the search area – a permutation.

Step 9. Combine virtual frogs of all memplexes into one group.

Step 10. If the conditions for the completion of the algorithm are not met, then go to Step 3.

Step 11. The last globally best virtual frog corresponds to a suboptimal problem solution.

Let us now describe this algorithm formally, taking into account the parameters.

The method parameters are as follows:

1) the number of classes of frogs Q $(Q \geq 2)$;

2) the number of elements *r* in each class (it is assumed that the sizes of the classes are the same and $r \geq 2$);

3) the maximum number of steps *K of the* algorithm;

4) the number *D of the* best frogs in the class, and $0 < D < r$.

In accordance with the specified parameters, the size *N* of the frog population (the set of feasible solutions) is determined by the formula $N = Qr$. In the initial step of the algorithm creates the initial population of frogs by generating random permutations $s^j = (i_{j1}, i_{j2}, .., i_{jn})$, $j = 1, 2, ..., N$.

The best permutation of the vertices in terms of the goal function is selected, which defines the permutation $s^* = (i_1, i_2, ..., i_n)$, and the value of the objective function is calculated $F(x^*)$ on this permutation:

Step k ($1 \le k \le K$). The set is ordered $P^{(k-1)}$ by the value of the objective function, that is $F(s^k) \ge F(s^{k-1}), \quad k = 2,3,...,N-1$. The population $P^{(k-1)}$ is divided into Q classes of the same cardinality r

$$P_q^{(k-1)} = \{s^{(qi)} \mid s^{(qi)} = x^j, \ j = q + (i-1)Q, \ i = 1,2,..,r, \ q = 1,2,...,q\}.$$

The best solution $s^* = s^1$ is determined by the value of the objective function for the entire population. In each class $P_q^{(k-1)}$, the "best" $s^{(q1)}$ and "worst" $s^{(qr)}$ are determined by the value of the objective function of the solution. In each class $P_q^{(k-1)}$, the positions (sequences of traversing the vertices of the graph) of frogs change with numbers from $D+1$ to r. For each value of the index $i \in \{D+1,2,...,r\}$ a new position of the i- th frog (the sequence of traversing the vertices) in the class with number q is determined according to the following rule: a random permutation s^c is calculated from the interval between the permutations $s^{(q1)}$ and $s^{(qr)}$ in the Kendall metric.

The permutation on the segment between $s^{(q1)}$ and $s^{(qr)}$ is built according to the rule: sequences $s^{(q1)}$ and $s^{(qr)}$ are viewed from left to right. At the next step, the smallest of the first elements of the sequences is selected and added to the new permutation. Then this element is removed from the permutations $s^{(q1)}$ and $s^{(qr)}$. For example, applying this operation to the permutations (2, 4, 7, 6, 1, 3, 5, 8) and (5, 8, 1, 3, 4, 2, 6, 7) gives the permutation (2, 4, 5, 7, 6, 1, 3, 8).

If $F(s^c) < F(s^{(qi)})$, then we assume $s^{(qi)} = s^c$. If $F(s^c) \ge F(s^{(qi)})$, then a random permutation s^c is chosen in the segment between $s^{(qr)}$ and $s*$. If $F(s^c) < F(s^{(qi)})$ then we assume $s^{(qi)} = s^c$. Otherwise, we choose a randomly generated permutation $s^{(qi)}$.

We assume $P^{(k)} = \bigcup_{q=1}^{Q} P_q^{(k-1)}$ and go to the next step of the algorithm.

The algorithm ends when the specified number of steps has been completed. The current permutation $s*$ determined at the last step is taken as the optimal solution to the problem.

Note that description is, the above algorithm s Resch was the problem of finding the optimal permutations of n elements in the set of all permutations with the objective function $F(s)$ which is defined on the set of permutations. In this case, the specific type of the objective function does not matter. Therefore, the above algorithm can be used to find suboptimal solutions to optimization problems on a set of permutations with arbitrary objective functions.

Numerical experiment. The weights of the graph edges were chosen randomly in the range [1,100]. These weights were considered as a measure of proximity for the respective vertices. The set of vertices of the graph was considered as a set of elements to be classified. A positive number was chosen randomly in the interval [0,1]. Linear orders (permutations) on the set of vertices were not adjusted using the Fisher-Yates shuffle algorithm [17].

The problems were solved using a local search algorithm, a random search method, evolutionary algorithms, and the method of mixed jumping frogs.

The comparison of algorithms was carried out in the following directions:

Record is the number of problems in a series where the algorithm turned out to be the best among the tested. Bord rating is the sum of the number of points scored on each problem in the series. For the first place in comparison, 5 points were assigned, for the second 4, for the third 3.

The results of the algorithm comparison are presented on Table 1.

Table 1. Results of applying different approaches.

Series (number of vertices)	Number of tasks	Algorithm search loc.		Random Search		Evolutionary algorithm		Jumping frog method	
		Record	Rating	Record	Rating	Record	Rating	Record	Rating
A 50	100	44	286	88	468	100	500	100	500
B 100	100	ten	221	0	348	100	500	100	500
H 500	100	0	212	0	280	94	394	100	500
D 1000	100	0	118	0	201	92	392	100	500

Conclusions. In this article, a method for finding optimal β-classifications based on two well-known metaheuristics was considered. A numerical experiment showed good results of the proposed algorithms in comparison with local and random search. This approach can be transferred practically without changes to other types of classifications, which are based on the concept of proximity of elements.

In addition to the metaheuristics proposed in the work, any other metaheuristics applicable to optimization problems on fragmentary structures can be considered in a similar way [10].

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METHOD OF LINES IN DISTRIBUTED PROBLEMS OF EXPERIMENTAL DATA PROCESSING

Gennady Shvachych, *Doctor of Science, National Metallurgical Academy of Ukraine, Dnipro, Ukraine, ORCID ID: https://orcid.org/0000-0002-9439-5511*
Nataliia Vozna, *Doctor of Technical Sciences, West Ukrainian National University, Ternopil, Ukraine, ORCID ID: https://orcid.org/0000-0002-8856-1720*
Ivashchenko Olena, *Candidate of Technical Sciences, National Metallurgical Academy of Ukraine, Dnipro, Ukraine, ORCID ID: https://orcid.org/0000-0003-4394-6907*
Oleksandr Bilyi, *Candidate of Technical Science, National Metallurgical Academy of Ukraine, Dnipro, Ukraine, ORCID ID: https://orcid.org/0000-0003-1234-5404*
Dmytro Moroz, *Master, Oles Honchar Dnipro National University, Dnipro, Ukraine, ORCID ID: https://orcid.org/0000-0003-2577-3352*

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ABSTRACT

In many cases, the mathematical support of non-stationary thermal experiments is based on methods for solving the inverse heat conduction problem (IHCP), which include boundary thermal conditions determination, identification of heat and mass transfer processes, restoration of external and internal temperature fields, etc. However, at present, the main field of the IHCP application remains the processing and interpretation of the results of the thermal experiments. It was here where the most considerable theoretical and applied successes were achieved in methods' effectiveness and the breadth of their practical use. This paper highlights the issues of mathematical modeling of multidimensional non-stationary problems of metallurgical thermophysics.

The primary research purpose aims at solving problems associated with identifying parallel structures of algorithms and programs and their reflection in the computers' architecture in solving a wide range of applied problems. Supercomputers are currently inaccessible due to the enormous cost and service price. In this regard, a real alternative is cluster-type computing systems by which the simulation results are covered in this paper.

Being a relatively new technology, cluster-type parallel computing systems are useful in solving a large class of non-stationary multidimensional problems, while allowing to increase the productivity and quality of computations. The software developed in this paper can be used to plan and process the results of a thermophysical experiment. The algorithms developed in the application program package are simply reconstructed to solve other coefficient and boundary problems of thermal conductivity. The developed algorithms for solving thermophysical problems are highly accurate and efficient: the test solution for IHCP with accurate input data coincides with the thermophysical features of the sample material. The developed software for processing the results of a thermophysical experiment is self-regulating. Moreover, it is quite merely tuned to the solution of others and, in particular, of boundary IHCP.

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Introduction. In metallurgical production, they face many diverse and interconnected processes. It includes heat transfer and mass exchange, hydrodynamic processes in melts, as well as a change in the substance aggregation state, deformation phenomena under power and thermal loads, etc. Most of these processes can be described based on differential equations of continuum mechanics, which reflect the objective laws of conservation of mass, momentum, and energy. In mathematical

terms, these are systems of multidimensional nonlinear differential equations that, like laws of chemistry and thermodynamics, describe interconnected processes, as well as their interaction.

Moreover, the practice of recent years shows that neither the intensification of the metallurgical production processes nor the constructive improvement of metallurgical equipment variety is possible without studying and analyzing the phenomena of heat transfer by methods of mathematical modeling [1, 2]. A theoretical study of the heat and mass transfer process is mainly based on their numerical simulation using computer technology. Besides, fundamental problems in the potentially endless increase of peak computer performance disappear with the development of cluster computing systems. Parallel computing systems are developing very fast, and with the advent of computing clusters [3, 4], parallel computing has become available to many. As a rule, mass processors, standard network technologies, and freely distributed software are used to build clusters. It was these circumstances that made the so-called big problems of metallurgical thermophysics [5 – 7] possible to solve.

At the same time, the problems arising in the development of parallel computing systems that meet unique features are, as a rule, paramount and require in-depth study and research [8, 9]. Indeed, distributed computer modeling covers the whole spectrum of modern computer technology: supercomputers, cluster computing systems, local and global networks. Besides, distributed modeling allows solving problems requiring huge processing time, integrate mathematical models that are processed on various (including geographically distant) computing systems.

In many cases, the mathematical support of non-stationary thermal experiments is based on methods for solving the inverse heat conduction problem (IHCP), which include boundary thermal conditions determination, identification of heat and mass transfer processes, restoration of external and internal temperature fields, etc. However, at present, the main field of the IHCP application remains the processing and interpretation of the results of the thermal experiments.

This paper highlights the issues of mathematical modeling of multidimensional non-stationary problems of metallurgical thermophysics.

The primary research purpose aims at solving problems associated with identifying parallel structures of algorithms and programs and their reflection in the computers' architecture in solving a wide range of applied problems.

Mathematical Formulation of Research Problem. When solving IHCP, it is first of all necessary to illuminate the controllability conditions of mathematical models (MM) that allow, by methods of mathematical modeling, bringing the system into a given thermal state using control actions. We will proceed from the fact that MM is known and includes several causal features, which we denote by the *R*-input parameters' vector. Let a discrete analog of MM and a computational algorithm be developed. The MM sensitivity to vector *R* variations, i.e., it is shown that the desired solution to a specific MM problem is determined not only by the functions of spatial coordinates and time but also by the *R*-input parameters' function. Thus, to evaluate the reliability of the obtained MM solution, it is necessary to study its behavior with variations in the input data. When studying the MM sensitivity, variations in input parameters are assumed to be given. Equally important are the formulation and methods of solving inverse problems, which essence is to evaluate the vector *R* input parameters from the actual information about the simulated system known from the experiment. The mathematical modeling process of this class of problems involves several stages.

First, the development of an algorithm and a computational program for solving the direct MM problem, the computational algorithm for solving that implements the transformation.

$$T = (x, t, R) \tag{1}$$

determining the MM temperature state vector as a function of independent variables and input parameters of the vector *R*.

Secondly, when solving IHCP as a quality criterion for identifying the parameters *R* on MM solutions, it is necessary to introduce into the algorithm a particular functional characterizing the model as a whole or the deviations between the measured $T_e(t_j)$ and the computed values of the state vector $T_p(t_j)$. Let us choose the standard mean square residual as deviation the measure.

$$(T_p, T_e) = (T_p - T_e)^2, \tag{2}$$

wherein T_p is the thermal state vector value computed by the MM model. The components of the $T_e(t_j)$ vector can be determined on a discrete set of points of a given domain of temperature function definition. As a rule, in practice, several such criteria are used for the model's quality assessment.

Thus, we have come to one of the promising directions in solving IHCP corresponding to their extreme formulation using well-known numerical methods of optimization theory. Considering that the computation of the vector *gradJ()* inherent in these methods is a serious mathematical problem, we show how this can be avoided. Note that if MM implements transformation (1), then at each step of such transformations, it is possible to compute the values of functional (2). It allows, by repeated variation of the vector *R* input parameters, constructing a sequence of changes in functional (2) that would include the point of its minimum. Thus, if this is feasible, then the IHCP solution is reduced to minimizing the function of many variables. This algorithm most looks merely for one variable of the vector *R*. The solving IHCP algorithm, in this case, includes separation of the interval containing the minimum functional point and the procedure for its refining. The update of the minimum coordinate can be implemented as follows. Suppose that the functional *J(R)* (2) has a sufficient analyticity margin concerning the vector *R* input parameters. Let us represent its value by a segment of the Taylor series near a minimum.

$$J_{p+\varepsilon_{k,}1}(R) = J_{p,1} + \varepsilon_R J_{p,2} + \varepsilon_R^2 J_{p,3} + ..., \tag{3}$$

wherein

$$\begin{aligned} \varepsilon_R &= \frac{R - R_p}{R_{p+1} - R_p} \in [-1,+1], \\ J_{p,2} &= (J_{p+1,1} - J_{p-1,1})/2, \\ J_{p,2} &= (J_{p+1,1} + J_{p-1,1} - 2J_{p,1})/2 \end{aligned} \tag{4}$$

are known Taylor components, and *p=1,2,3, ...* are the numbers of grid nodes.

Having saved three terms in (3), differentiating concerning $\mathcal{E}_R$, and equating to zero, we construct the interpolation formula

$$R = R_p - \frac{(R_{p+1} - R_p)}{2} \cdot \frac{J_{p,2}}{J_{p,3}}, \tag{5}$$

wherein all the notations correspond to those adopted above. Thus, the IHCP solution from this class of problems reduces to separating the minimum and its refinement by iterations according to formula (5). This algorithm is tested below on solutions of coefficient IHCP.

Construction Features of the Controlled MM for the Coefficient IHCP Problem. Let us consider the one-dimensional problem of unsteady heat conduction described by the quasilinear equation.

$$C_{UV}(T)\frac{\partial T}{\partial \tau} = \frac{1}{x^K}\frac{\partial}{\partial x}\left[x^K\left(\lambda(T)\frac{\partial T}{\partial x}\right)\right], x \in [0,1], \tau \in [0,\infty), \tag{6}$$

wherein

$$\begin{aligned} &\tau = a_0 t / L^2, a_0 = \lambda_0 / C_{\upsilon 0}, \\ &x = x / L, C_\upsilon = C_\upsilon / C_{\upsilon 0}, \\ &\lambda = \lambda / \lambda_0, k = \overline{0,1,2}, \end{aligned} \tag{7}$$

are dimensionless input data, *k* is a parameter of the sample (plate, cylinder, and ball) shape.

Equation (6), after time discretization, is transformed at grid domain nodes (*p=1,2,…,m_x-1*) into an ordinary differential equations system of a two-point type.

$$T''_{p+\varepsilon_x,1}(\varepsilon_x) + 2A_p T'_{p+\varepsilon_x,1}(\varepsilon_x) - B_p T_{p+\varepsilon_x,1}(\varepsilon_x) = B_p TO_{p+\varepsilon_x,1}(\varepsilon_x), \tag{8}$$

wherein

$$\left.\begin{aligned} A_p &= \frac{1}{2}\left(\frac{\lambda_{p,2}}{\lambda_{p,1}} + k\frac{Dx1}{x_p}\right) \\ B_p &= \frac{Dx1}{Dt1}\frac{CV_{p,1}}{\lambda_{p,1}} \end{aligned}\right\}. \tag{9}$$

The functions $T_{p+\varepsilon_{x,}1}(\varepsilon_x), TO_{p+\varepsilon_{X},1}(\varepsilon_x)$ in (9) are assigned to the current and previous time layers, respectively.

The solution of the investigated differential equation according to the direct method is presented in an analytical form by nodes

$$T_{p+\varepsilon_x,1}(\varepsilon_x) = T^*_{p+\varepsilon_x,1}(\varepsilon_x) + C_p e^{\beta_1 \varepsilon_x} + D_p e^{-\beta_2 \varepsilon_x}, \tag{10}$$

wherein

$$\beta_1 = \Omega_p - A_p, \quad \beta_2 = \Omega_p + A_p, \quad \Omega_p = \sqrt{A_p^2 + B_p}, \tag{11}$$

are the roots of the characteristic equation;

C_p, D_p are the integration constants;

$T^*_{p+\varepsilon_{X1}}(\varepsilon_X)$ is a particular solution to the inhomogeneous equation (8).

The final sub-node solution to this problem takes the following form

$$T_{p+\varepsilon_x,1}(\varepsilon_x) = T^*{}_{p+\varepsilon_x,1}(\varepsilon_x) + F1\frac{e^{-\beta_1(1-\varepsilon_x)}}{Det}(1-e^{-2\Omega_p(1+\varepsilon_x)}) + \\ + F2\frac{e^{-\beta_1(1+\varepsilon_x)}}{Det}(1-e^{-2\Omega_p(1-\varepsilon_x)}), \tag{12}$$

wherein

$$F1 = (T_{p+1,1} - T^*_{p+1,1}), F2 = (T_{p-1,1} - T^*_{p-1,1}), Det = (1-e^{-4\Omega_p}) \tag{13}$$

are the grid complexes.

Setting in (12) $\mathcal{E}_x=0$, we obtain MM algebraic analog in the form of a system of linear differential equations of a tridiagonal structure

$$C_p T_{p+1,1} - T_{p,1} + D_p T_{p-1,1} = f_{p,1}, \quad p = \overline{1,2m-1}, \tag{14}$$

wherein

$$\left.\begin{aligned} C_p &= \frac{e^{-\beta_1}}{1+e^{-2\Omega_p}} \\ D_p &= \frac{e^{-\beta_2}}{1+e^{-2\Omega_p}} \\ f_{p,1} &= (C_p T^*_{p+1,1} - T^*_{p,1} + D_p T^*_{p-1,1}) \end{aligned}\right\}. \tag{15}$$

The quadratic dependence of the argument $TO_{p+\varepsilon_{X1}}(\varepsilon_X)$ concretizes the form of the initial function $\mathcal{E}_x$

$$TO_{p+\varepsilon_x,1}(\varepsilon_x) = TO_{p,1} + \varepsilon_x TO_{p,2} + \varepsilon^2{}_x TO_{p,3}, \tag{16}$$

wherein

$$\left.\begin{aligned} TO_{p,2} &= \frac{1}{2}(TO_{p+1,1} - TO_{p-1,1}) \\ TO_{p,3} &= \frac{1}{2}(TO_{p+1,1} + TO_{p-1,1} - 2TO_{p,1}) \end{aligned}\right\}. \tag{17}$$

Considering these dependencies, particular solution of inhomogeneous equation (8), which is included in the MM (14) in an implicit form, takes following form

$$TO^*_{p+\varepsilon_x,1}(\varepsilon_x) = M_0 + \varepsilon_x M_1 + \varepsilon^2{}_x M_2, \tag{18}$$

wherein

$$\left.\begin{aligned} M_0 &= TO_{p,1} + b_1 TO_{p,2} + 2b_2 TO_{p,3} \\ M_1 &= TO_{p,2} + b_1 TO_{p,3} \\ M_2 &= TO_{p,3} \\ b_1 &= 2\frac{A_p}{B_p}, b_2 = 4\frac{A_p^2}{B_p^2} + \frac{1}{B_p} \end{aligned}\right\}. \tag{19}$$

The solution of linear algebraic equations system (14) for given input data is entirely simply implemented by the sweep method. Thus, we can assume that we developed the first MM being necessary to solve the coefficient IHCP in the above (extreme) statement. Let us designate it as Model 1. We should also add its gradient analog to the (temperature) MM (14). By differentiating function (12) $\mathcal{E}_x$ concerning and setting $\mathcal{E}_x=0$, we construct the gradient Model 2

$$T_{P,2}(\varepsilon_x)_{\varepsilon_x=0} = \left\{T^*_{P,2}(0) + F1\frac{\ell^{-\beta_1}}{Det}\left[\beta_1 + \beta_2\ell^{-2\Omega p}\right] - F2\frac{\ell^{-\beta_2}}{Det}\left[\beta_2 + \beta_1\ell^{-2\Omega p}\right]\right\}, \tag{20}$$

wherein the function $T^*_{p+\varepsilon 2}(\varepsilon_X)$ is computed by the formula

$$T^*_{p+\varepsilon_x,2}(\varepsilon_X) = M_1 + 2\varepsilon_X M_2. \quad (21)$$

Thus, the identification MM, which includes Model 1 (14) and Model 2 (20), allows formulating a solution to the coefficient IHCP in an extreme setting according to the scheme described above.

The proposed approach is implemented as a package of application programs.

The Solution of the Test Coefficient IHCP Using Mathematical Modeling. As a test problem let us consider a cylindrical sample made of a material with thermophysical properties [16] (coke from gas coal p. 41, Table 42-molded coke):

$$\lambda = 0.161 + 0.024 \cdot 10^{-2} \cdot T$$
$$C = 1.281 + 0.208 \cdot 10^{-2} \cdot T, \quad (22)$$

The density of coke from gas coal $p = 1912, kg/m^3$. With such thermophysical properties, we simulated the temperature field of a cylindrical shape sample *(k=1)*. For given time-linear temperature change at sample boundary $(TL = 20 + 100 \cdot \tau)$, the temperature field for a particular time moment $\tau = a_0 t / R^2 = 0.5$, wherein $a_0 = \lambda_0 / p\, c_0 (\lambda_0 = 1, c_0 = 1)$, shown in Fig. 1 - 3.

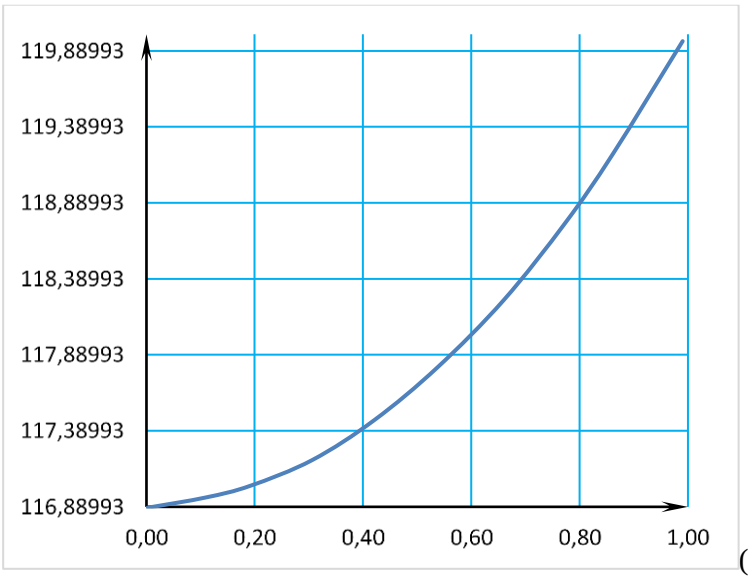

Fig. 1. The change in temperature over the at time moment $\tau = \tau_1 = 0,5$

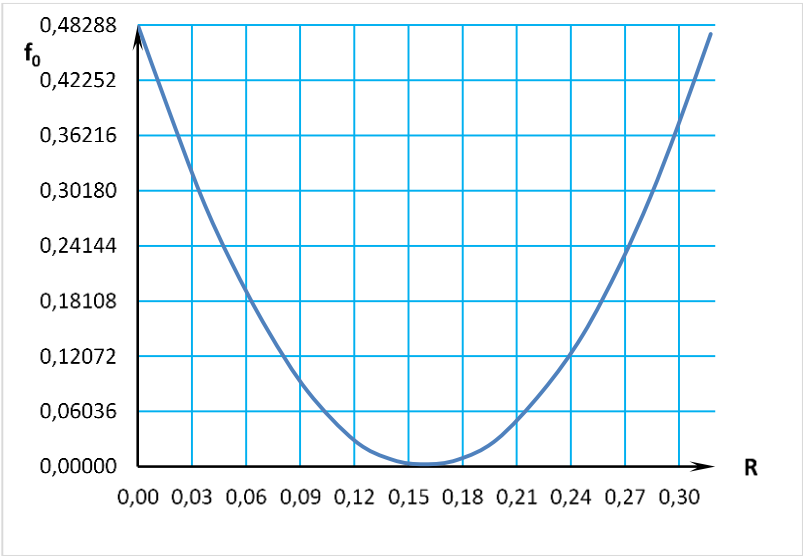

Fig. 2. The solution of the coefficient cross-section of the sample IHCP with $R = \lambda$

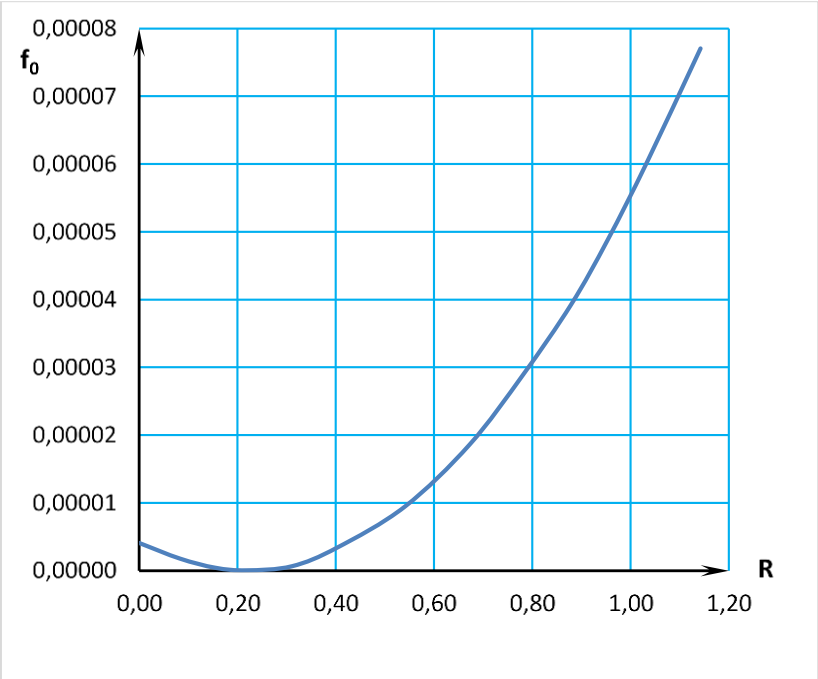

Fig. 3. The solution of the coefficient IHCP with $R = a$ *with control relative to the coefficient of thermal diffusivity*

The coefficient exact values of thermal conductivity and thermal diffusivity are respectively equal $\lambda(f_2) = 0.166, a(f_2) = 0.054$, wherein f_2 is the temperature change in the second node along the cross-section of the sample. The minimum residuals presented in Fig. 2, 3 exactly correspond to these values.

Conclusions. In many cases, the mathematical support of non-stationary thermal experiments is based on methods for solving the inverse heat conduction problem (IHCP), which include boundary thermal conditions determination, identification of heat and mass transfer processes, restoration of external and internal temperature fields, etc. However, at present, the main field of the IHCP application remains the processing and interpretation of the results of the thermal experiments. It was here where the most considerable theoretical and applied successes were achieved in methods' effectiveness and the breadth of their practical use. This paper highlights the issues of mathematical modeling of multidimensional non-stationary problems of metallurgical thermophysics.

The primary research purpose aims at solving problems associated with identifying parallel structures of algorithms and programs and their reflection in the computers' architecture in solving a wide range of applied problems.

Supercomputers are currently inaccessible due to the enormous cost and service price. In this regard, a real alternative is cluster-type computing systems by which the simulation results are covered in this paper.

Being a relatively new technology, cluster-type parallel computing systems are useful in solving a large class of non-stationary multidimensional problems, while allowing to increase the productivity and quality of computations.

The software developed in this paper can be used to plan and process the results of a thermophysical experiment. The algorithms developed in the application program package are simply reconstructed to solve other coefficient and boundary problems of thermal conductivity.

The developed algorithms for solving thermophysical problems are highly accurate and efficient: the test solution for IHCP with accurate input data coincides with the thermophysical features of the sample material.

The developed software for processing the results of a thermophysical experiment is self-regulating. Moreover, it is quite merely tuned to the solution of others and, in particular, of boundary IHCP.

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EDGE COLORING OF CACTUS GRAPHS WITH GIVEN SPECTRUMS

Albert Khachik Sahakyan,
Chair of Discrete Mathematics and Theoretical Informatics, Faculty of Informatics and Applied Mathematics, Yerevan State University, Armenia

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ABSTRACT

An edge-coloring of a graph G is a coloring of the graph edges with integers such that the colors of the edges incident to any vertex of G are distinct. For an edge coloring α and a vertex v the set of all the colors of the incident edges of v is called the spectrum of that vertex in α and is denoted by $S_\alpha(v)$. We consider the case where the spectrum for each vertex v is provided $S(v)$, and the problem is to find an edge-coloring α such that for every vertex v, $S_\alpha(v) = S(V)$. We provide an $O(N^2)$ algorithm that finds such an edge-coloring for cactus graphs that satisfies all the restrictions. If it is impossible to have an edge-coloring that satisfies the restrictions of the spectrums the algorithm will tell that too.

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Introduction. All graphs considered in this paper are undirected (unless explicitly said), finite, and have no loops or multiple edges. For an undirected graph G, let $V(G)$ and $E(G)$ denote the sets of vertices and edges of G, respectively. The degree of a vertex $v \in V(G)$ is denoted by $d_G(v)$.

A cactus is a connected graph in which any two simple cycles have at most one vertex in common. Equivalently, it is a connected graph in which every edge belongs to at most one simple cycle. Fig. 1 illustrates different examples of cactus and non-cactus graphs.

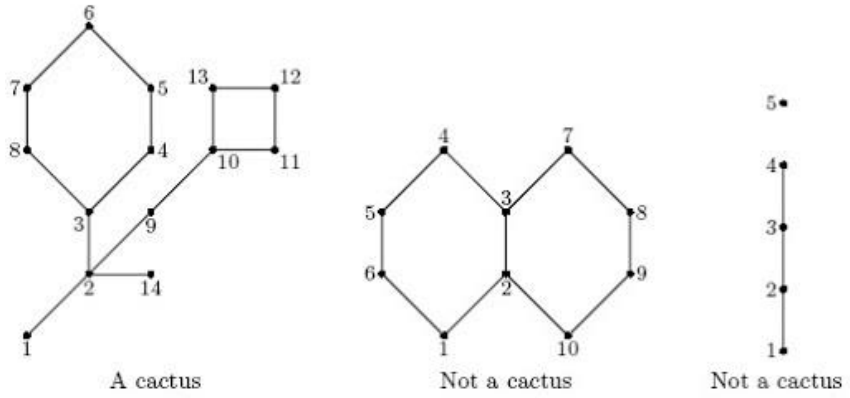

Fig. 1. Example of cactus and non-cactus graphs.

An edge-coloring of a graph G is a coloring of the graph edges with integers such that the colors of the edges incident to any vertex of G are distinct. For an edge coloring α and a vertex v the set of all the colors of the incident edges of v is called the spectrum of that vertex in α and is denoted by $S_\alpha(v)$.

A cut vertex is any vertex whose removal increases the number of connected components [1]. Any connected graph decomposes into a tree of biconnected components called the block-cut tree of the graph [9] (pg. 36). Cactus is a connected graph in which every block is an edge or a cycle [1] (pg. 160).

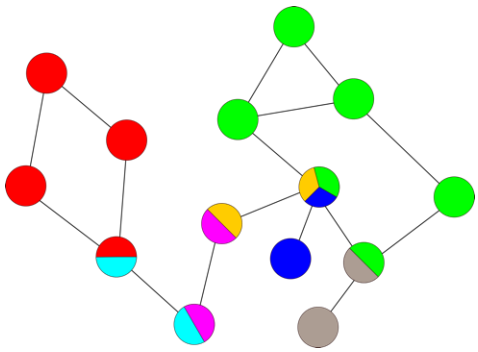

Fig. 2. Each color corresponds to a biconnected component. Multi-colored vertices are cut vertices, and thus belong to multiple biconnected components.

Finding a coloring for given spectrums were researched in different studies. In [2] a solution for the simplified version of this problem was provided for trees when the restrictions are on the spectrums, the restrictions are strict, and all the spectrums contain the color 1. In [3] another limited version was considered for trees where each vertex had at most one interval of forbidden colors. In [4] and [5] it was shown that for bipartite graphs with maximum degree equal to 3 and with strict restrictions on spectrums the problem of finding a coloring that meets the restrictions is an NP-complete problem. In [6] another problem with restrictions is considered for bipartite graphs where the restrictions are provided for one "part" of the bipartite graph. Finding a coloring for given spectrums is important for finding interval t-colorings which was first introduced by Kamalian and Asratian in [7]. When the restrictions on spectrums are intervals of integers then finding an edge-coloring is the same as finding an interval edge coloring. Finding an interval edge coloring for cactus graphs was researched in [8] but for bipartite cactuses.

An $O(N^2)$ algorithm for edge coloring with given spectrums

Here we will provide an algorithm that finds an edge coloring for a cactus where the spectrums are given for all the vertices. The algorithm will also detect if it is impossible to find a coloring that satisfies all the restrictions. When saying that given the spectrum $S(v)$ for a vertex v in the graph G we will understand that a strict restriction is provided for the vertex v such that $|S(v)| = d_G(v)$ and we are interested in finding an edge-coloring α such that $S_\alpha(v) = S(v)$

Problem: Given a cactus graph C and for each vertex v the spectrum $S(v)$ is given with $|S(v)| = d_C(v)$. Find an edge-coloring α such that $S_\alpha(v) = S(v)$ for all v or find out that it's impossible to find such coloring.

Lemma 1: If there is a proper edge coloring for given spectrums and there is an edge $(u, v) \in E(G)$ such that $|S(u) \cap S(v)| = 1$ then the color of the edge (u, v) should be the single element from $S(u) \cap S(v)$.

Imagine in the final coloring α the edge (u, v) has the color c ($c = \alpha(u, v)$), it means that $c \in S(u)$ and $c \in S(v)$ hence $c \in S(u) \cap S(v)$ but since $|S(u) \cap S(v)| = 1$ it means $S(u) \cap S(v) = \{c\}$ hence if an edge-coloring exists it should color the edge (u, v) with the color c.

Lemma 2: If for some edge $(u, v) \in E(G)$, $|S(u) \cap S(v)| = 0$ then there is no edge-coloring that satisfies the spectrum restrictions.

We will prove by contradiction. Assume there was an edge-coloring α that satisfies all the restrictions. Let $c = \alpha(u, v)$, it means that $c \in S(u)$ and $c \in S(v)$ hence $c \in S(u) \cap S(v)$ which means $|S(u) \cap S(v)| \geq 1$ which is a contradiction.

Lemma 1 and Lemma 2 give us a constructive approach for finding an edge-coloring. If there is an edge (u, v) for which $|S(u) \cap S(v)| = 0$ then it's impossible to find an edge-coloring, otherwise if there is an edge (u, v) such that $|S(u) \cap S(v)| = 1$ we will color the edge (u, v) with the color c from $S(u) \cap S(v)$, remove the edge (u, v) and remove the color c from $S(u)$ and $S(v)$. Removing the edge (u, v) would either make the graph disconnected in which case we would solve

for each graph component separately or we would end up with a smaller graph because the number of edges decreases.

This means that we can assume there is no edge (u, v) with $|S(u) \cap S(v)| = 1$ hence for each edge (u, v), $|S(u) \cap S(v)| \geq 2$.

Lemma 3: If for each edge (u, v), $|S(u) \cap S(v)| \geq 2$ then there is no leaf vertex (a vertex with degree equal to 1).

If there existed a vertex v with $d_G(v) = 1$ that was connected to a vertex u, then $|S(v)| = 1$ and $2 \leq |S(u) \cap S(v)| \leq |S(v)| = 1$ which is a contradiction.

Lemma 4: In a cactus C with no leaf vertices and $|V(C)| \geq 3$ there is always a cycle for which all the vertices on that cycle except maybe one vertex have degree 2.

Since there are no leaf vertices and $|V(C)| \geq 3$ then there is at least one cycle. Let's consider the block-cut tree of the cactus C. Fig 3 illustrates an example of such cactus on the left and its respective block cut tree on the right. In the image the vertex 2 is the cut vertex c_1 , the vertex 8 is the cut vertex c_2 etc.

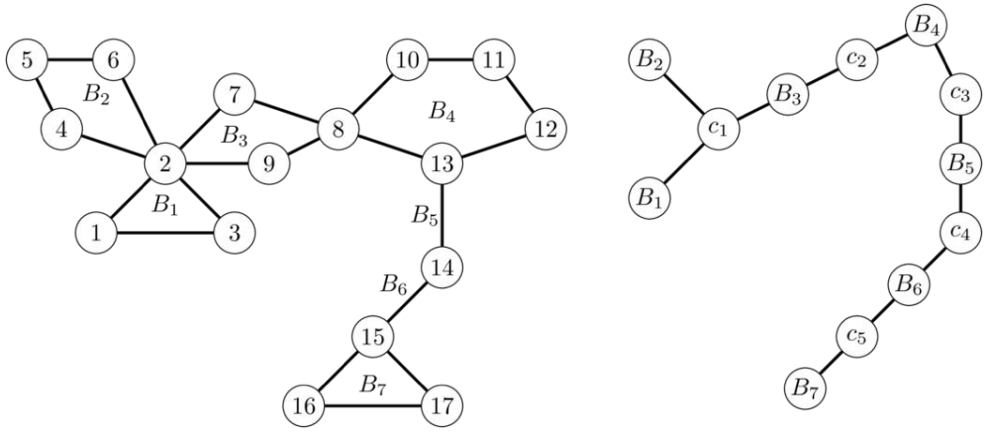

Fig 3. A cactus with no leaf vertices and its block-cut tree.

Since the block-cut tree is a tree, it has a leaf vertex which is a block because a cut vertex should be connected to at least two blocks. Let's suppose the block B is a leaf in the block-cut tree. The block B consists of vertices $u_1, u_2, \dots, u_k$. Each block of a cactus is either an edge or a cycle but since in our case the cactus has no leaf vertices it means the block B is a cycle (otherwise it would be an edge that connects a leaf vertex in the cactus). Since B is a leaf vertex in the cut-vertex tree it means it contains at most one cut vertex which means there can be at least one vertex in the cycle B that has degree more than 2. All the other vertices will have degree 2 which was required to prove in this lemma.

We already managed to transform our original cactus to a set of cactuses where for each edge (u, v), $|S(u) \cap S(v)| \geq 2$ and hence by Lemma 3 there are no leaf vertices.

Now imagine we have a cactus C that has no leaf vertices and for each edge (u, v), $|S(u) \cap S(v)| \geq 2$. From Lemma 4 we can find a cycle $C_1 = (u_1, u_2, \dots, u_k)$ such that at most one vertex has degree greater than 2. Let that vertex be the vertex u_1, then $d_C(u_2) = 2, \cdots, d_C(u_k) = 2$ and $(u_1, u_2) \in E(C), (u_2, u_3) \in E(C), \cdots, (u_{k-1}, u_k) \in E(C)$ and $(u_k, u_1) \in E(C)$. Since this is a cycle, it means $k \geq 3$. Now, we know that for each (u_i, u_{i+1}) edge $(2 \leq i \leq k-1)$ $|S(u_i) \cap S(u_{i+1})| \geq 2$ and on the other hand $|S(u_i)| \leq d_C(u_i) = 2$, $|S(u_{i+1})| \leq d_C(u_{i+1}) = 2$ hence $|S(u_i)| = 2$ and $|S(u_{i+1})| = 2$ and $S(u_i) = S(u_{i+1})$. Which means for all the vertices u_i $(2 \leq i \leq k)$ the spectrums are the same and consist of two colors. Let's suppose these colors are a and b it means for all the edges on this cycle we should color only with colors a or b and the colors should be interchangeable. It means that if k is odd it will be impossible to satisfy the requirements, and if k is even we can freely color interchangeably and it does not matter which edges we will color with a and which edges we will color with b since we are going to remove both the color a and the color b from the spectrum $S(u_1)$. Fig 4. illustrates the two cases for odd $(k = 2 * m + 1)$ and even $(k = 2 * m)$ cycles. After the coloring we can remove all the edges of the cycle and also remove the colors a and b from all the spectrums of the vertices in this cycle. This way we managed to reduce the problem to smaller problems for each new component.

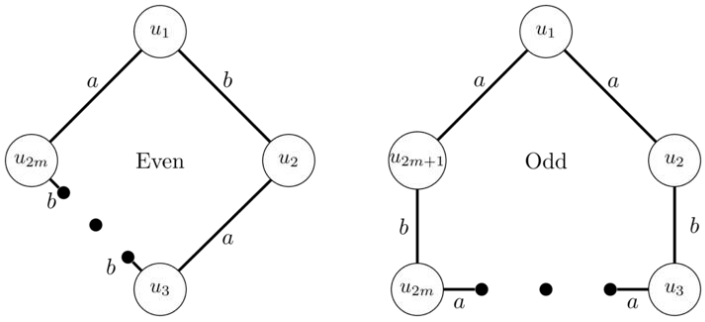

Fig. 4. The coloring of the cycle for the odd and even number of vertices.

For a cactus C and spectrums S the algorithm of constructing edge coloring α is the following:

- *Step1:* If there is no edge in C then we found the edge coloring that meets all the restrictions and we can terminate the algorithm with the answer α.
- *Step2:* If there is an edge $(u, v) \in E(C)$ with $|S(u) \cap S(v)| = 0$ then it is impossible to find a coloring and we can terminate the algorithm.
- *Step3:* If there is an edge $e = (u, v) \in E(C)$ with $|S(u) \cap S(v)| = 1$ with the color $c \in S(u) \cap S(v)$ then we assign $\alpha(e) = c$, remove the edge e from C, remove the color c from $S(u)$ and $S(v)$ and go to *Step1*.
- *Step4:* Let $e = (u, v)$ be an arbitrary edge that we did not remove yet.
  - In the connected component that contains this edge we find a cycle for which all the vertices except maybe one, have degree equal to 2.
  - We can do it by checking all the cycles in the component since finding all the cycles of a cactus can be done in $O(N)$.
  - Let $u_1, \dots, u_k$ be that cycle where the vertex u_1 does not need to have degree equal to 2. If k is odd then it's impossible to find a coloring and we can terminate the algorithm. If k is even $(k = 2 * m)$ let $S(u_2) = \{a, b\}$ then for the edges (u_{2*i}, u_{2*i+1}) with $1 \le i \le m - 1$ and for the edge (u_{2*m}, u_1) we assign $\alpha(u_{2*i}, u_{2*i+1}) = a$, $\alpha(u_{2*m}, u_1) = a$ and for the edges (u_{2*i-1}, u_{2*i}) with $1 \le i \le m$ we assign $\alpha(u_{2*i-1}, u_{2*i}) = b$.
  - We remove the edges of the cycle from C, remove the colors a and b from $S(u_i)$ for $1 \le i \le k$ and go to *Step1*.

If $N = |V(G)|$ this can give us a simple $O(N^2)$ algorithm, since for cactuses $|E(C)| = O(N)$ and we removed an edge or a cycle after every iteration and finding such an edge or a cycle can be done in $O(N)$.

Conclusions. We provided an $O(N^2)$ algorithm for finding an edge-coloring of a cactus for the given spectrums on the vertices. The algorithm can be used for trees too since trees are special case of cactus graphs. When each spectrum is an interval then the coloring will be an interval edge coloring.

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ECOLOGY

BIOREMEDIATION OF SOILS CONTAMINATED WITH HEAVY METALS

R. Z. Uridia, *Ph.D., Candidate of chemical sciences, Iv. Javakhishvili Tbilisi State University, P. Melikishvili Institute of Physical and Organic Chemistry, Tbilisi, Georgia*
N. A. Kavtaradze, *Ph.D., Candidate of chemical sciences, Iv. Javakhishvili Tbilisi State University, P. Melikishvili Institute of Physical and Organic Chemistry, Tbilisi, Georgia*
K. N. Kochiashvili, *Ph.D., Candidate of chemical sciences, Iv. Javakhishvili Tbilisi State University, P. Melikishvili Institute of Physical and Organic Chemistry, Tbilisi, Georgia*
M. A. Stephanishvili, *Ph.D., Candidate of chemical sciences, Iv. Javakhishvili Tbilisi State University, P. Melikishvili Institute of Physical and Organic Chemistry, Tbilisi, Georgia*
I. I. Mikadze, *Ph.D., Candidate of chemical sciences, Iv. Javakhishvili Tbilisi State University, P. Melikishvili Institute of Physical and Organic Chemistry, Tbilisi, Georgia*
L. A. Dolidze, *Ph.D., Candidate of chemical sciences, Iv. Javakhishvili Tbilisi State University, P. Melikishvili Institute of Physical and Organic Chemistry, Tbilisi, Georgia*
T. A. Dgebuadze, *Scientist, Iv. Javakhishvili Tbilisi State University, P. Melikishvili Institute of Physical and Organic Chemistry, Tbilisi, Georgia*

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ABSTRACT

Waste generated due to the growth of the modern industry is undergoing natural disposal in the environment for a long period of time. A special danger is caused by heavy metals that do not undergo biodegradation. Known purification methods of soils are not always effective and profitable. Correct selection of soil remediation methods contaminated with heavy metals ensures effective cleaning and restoration of soils. For this purpose, selecting representatives of various taxonomic groups of microorganisms binding heavy metals in the soil is carrying out. A complex method of purification of soils contaminated with have metals is being developed. Modified forms of humic acids were developed, geochemical barriers using local clays were created. Works to biostimulate local microorganisms required for bioremediation of soils contaminated with heavy metals are conducted. Remediation and increasing the fertility of soils contaminated with heavy metals are necessary for the prevention of further penetration of these metals into agricultural crops.

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Introduction. Research of contamination sources of environment and their elimination is the most important problem. Waste generated due to the growth of the modern industry is undergoing natural disposal in the environment for a long period of time. In this regard, a special danger is caused by heavy metals that do not undergo biodegradation. Significant amounts of heavy metals accumulate in microorganisms and plant biomass, then by trophic chain enter organism of animals and humans, and negatively affect their activity. It should be mentioned, that the degree of contamination is

especially high in regions where the industry is highly developed. Heavy metals pollution causes changes in natural biocenosis. They cause inhibition of activity in some microorganisms.

There are several sources of heavy metal contamination in Georgia. Arsenic, copper, lead, cadmium, strontium, strontium, nickel, chrome belong to the main pollutants. The map of pollution with heavy metals of the territory of Georgia is drawn up, the level of contamination and polluted places are identified. The most contaminated places with radionuclides are identified (the southern part of Georgian Black Sea Coast of Adjara and Ozurgeti regions). It is necessary to determine the initial data of heavy metals concentration using modern technologies [1]. Thus, the development of effective methods for purification the environment from heavy metals contamination is relevant.

Different technologies to restrict the migration of heavy metals into the soil are widely used in the modern world. This can be achieved by immobilizing heavy metal ions on various solid surfaces, using ameliorants or stabilizers. For this purpose, it is effective to use natural and synthetic phosphates [2]. There are phosphorus-containing deposits in Georgia, but in this case, we did not consider their application appropriate due to unprofitability. Some basic oxides, hydroxides and sulfides can be used as ameliorators and stabilizers. Effective and accessible ameliorant has not been determined yet. It should be noted that it is difficult to find a universal ameliorator that can effectively immobilize all possible heavy metals in the soil. We are actively conducting research in this direction.

Heavy metals mainly accumulate in the upper layers of the soil. This depends on the mechanical and mineral composition of the soil. The degree of accumulation of heavy metals is especially high in soils with high humus content and heavy granulometric composition, as well as in dry soils rich with montmorillonite clays. The migration of heavy metals in such soils is restricted.

The rate of soil purification from heavy metals depends on the rate of decay of radioactive substances and the ability of these metal ions to migrate into the soil. Purification of soils contaminated with heavy metals is implemented using chemical and microbiological technologies [3, 4].

Heavy metals are divided into three groups according to the negative effect on the environment. The most hazardous: Hg, Pb, Zn, Cd, etc.; Medium hazardous: Ni, Cu, Cr, Sb, Co, and less harmful Mn, Sr. Heavy metals are also distinguished by their ability to migrate into soils. Heavy metals are found in soils in the form of free ions, as well as water-soluble inorganic and organic complexes.

Known methods of remediation of soils polluted with heavy metals are divided into three groups: restriction, *ex-situ* and *in situ*. The restriction method of heavy metals distribution in soils includes the creation of geo-barriers, mechanical insulation and sealing. This ensures the binding of contamination in a specific location and prevents the introduction of highly toxic heavy metal ions into the natural environment. *Ex-situ* method includes physical separation of soil contamination, leaching and pyrometallurgical treatment of soil. The application of this method is limited since its implementation requires an appropriately arranged area. The third group of existing cleaning methods includes the creation of isolated water-permeable barriers, electrokinetic treatment, soil washing, biological leaching, and phytoremediation.

Proper selection of these methods ensures effective soil purification and restoration. It should be noted that in the recent past, only phytoremediation has been used among biomethodes. To reduce soil contamination toxicity, mobile ions can be leached and other heavy metals converted to non-mobile forms. It should be noted, that this may result in the formation of more toxic compounds.

These technologies of restriction of heavy metals distribution in the soils are not able to completely remove hazardous xenobiotics but stabilize them in areas of contamination. The method of soil washing with organic acids and synthetic surfactants is based on chemical-technological processes. During this, such aggressive reagents are used that significantly worsen the existing ecological situation.

Research results. Described purification methods of soils are not always effective and profitable an effective and environmentally safe method of cleaning soils from heavy metals is the use of microorganisms. It is known that many microorganisms are not subjected to severe toxic effects and it is possible to increase their resistance. For this purpose, the selection of local bacteria and fungi able to bind heavy metals in the soils is conducted. Using representatives of different taxonomic groups of microorganisms is possible. Some microorganisms during life activity reduce water-soluble sulphates of certain heavy metals (Cd, Pb, Cu) into water-insoluble sulphides. This makes possible to bind pollutants in the soil that subsequently be washed away with sewage.

Synthetic surfactants are environmentally hazardous, highly toxic substances with a low level of biodegradation. They also actively accumulate in the soil

biocenosis. Therefore, treatment of soils contaminated with heavy metals using ecologically safe biogenic surfactants of bacterial origin is perspective. Biosurfactants have the ability to form complex compounds with metal ions. The active surface of surfactants promotes and facilitate the desorption of contaminants by microbial cells. Therefore, they are effective agents in the bioremediation of soils contaminated with heavy metals. Selection of biosurfactants with environmentally safe and metallo-chelating abilities is necessary. Their similarity with the type of contamination, high mobility in the soil and long-existing ability should be considered. Biosurfactants synthesized by microorganisms fully meet these requirements. They have almost completely replaced the synthesized analogues. Natural surfactants are biodegradable and characterized by low toxicity and high activity in extreme conditions [5, 6].

Bacteria of the genus Rhodococcus have high oxidizing activity, the ability to accumulate ions of heavy metals and synthesize non-toxic biosurfactants. This promotes to the restoration of soils contaminated with heavy metals. The leaching of heavy metals in the soils by means of *Rhodococcus*-biosurfactants is explained by the formation of a stable chelating complex between the metal and the biosurfactant molecule. Using immobilized *Rhodococcus* promotes the isolation of Ni 2+ from the soil. Despite various immobilization methods, induced *Rhodococcus* retain high functional activity during bioreduction. Their introduction into contaminated soils activates soil respiration processes, which is explained by the biodegradation of hydrocarbons by these species of bacteria. It is established that the number of *Rhodococcus* in the purified soil decreases and reaches the limit of the norm. This proves their ecological safety.

At the first stage of the experiment conducted by us, certain strains of microorganisms were selected for bioremediation, artificial contamination of soils with aqueous solutions of heavy metal salts have been done and soil acidity was determined. Correction of soils acidity with a slaked lime is performed, which helps to prolong soil fertility as well [7].

For absorption of heavy metals modified natural sorbents are used. As components of geochemical barriers, local clay minerals kaolinite and montmorillonite are used. That promotes the deposition of xenobiotics and prevent the transfer of contamination into groundwater [8]. Natural sorbents have been modified with derivates of humic acids extracted from peat, while inorganic acids and salts have been used to increase the sorption capacity. Humic acids were modified with iron ions Fe^{2+}, which decreased the solubility of heavy metals in humic acid. This prevents the formation of soluble and consequently mobile complexes of metals. It should be noted that modified humic acids are effective sorbents for Pb^{2+} and Cu^{2+} ions, whereas in the case of Zn^{2+} the degree of sorption is low.

Optimal conditions for biostimulation of local microorganisms selected for the accumulation of xenobiotics have been selected.

The humidity of the model contaminated samples was 40%, temperature 22-25°C. After 14 days from artificial contamination, local dry sorbents (kaolinite and montmorillonite) were introduced into the soils. During the studies, the watering and loosening of soil samples were carried out regularly once a week. Contaminated soil samples without sorbents are taken as a control. The quantity and quality of microflora have been studied using traditional microbiological methods [9].

We conducted quantitative and qualitative microbiological analyses of non-contaminated and artificially contaminated soil samples. 10 groups of microorganisms were isolated from the soil sample. The number of microorganisms was determined by sowing the soil suspension in the nutrient area. The results were evaluated on a petri dish, the calculation was made on 1 g of soil. At this stage of the study, remediation was performed by means of *Azotobacter* and *Nitrobacter*, representatives of the *Nitrogen-fixing bacteria* genus since their percentage distribution in the studied soils compare to other groups of microorganisms was high. Quantitative and qualitative analysis has shown that in the initial stage, a quantitative reduction of microorganisms in artificially contaminated soils is observed, and during the remediation process, their gradual recovery is noticed. It should be noticed that the low content of oligocarbophiles in contaminated soils is a sign of their low fertility and during the experiment, their number has increased (Table 1).

Table 1. Quantitative content of microorganisms (%) per 1 g of soil

Microorganism	Quantitative content of microorganisms (%) per 1 g of soil	
	Artificially contaminated soil before remediation	Soil in the early stage of remediation
Nitrate-reducing	16.1	21.25
Denitrifying bacteria	12.2	18.5
Cellulose-destroying	9	8
Nitrogen-fixing bacteria	20.1	27.05
Ammonifiers	4.2	2.5
Actinomycetes	18.6	9.75
Fungi / yeast	8.4	5.25
Nitrifiers I	7.4	3.70
Nitrifiers II	2	1
Oligo Carbophils	2	3

As can be seen from the table, there are some changes between soil artificially contaminated with heavy metals before remediation and soil at an early stage of remediation. The number of actinomycetes and fungi have been increased in soils contaminated with heavy metals, although the quantity of nitrogen-fixing bacteria has not changed much [10].

Currently, works for biostimulation of local microorganisms needed for bioremediation of soils contaminated with heavy metals is carrying out. Recommendations for soil remediation based on the microbiological analysis of the studied soil samples will be developed. Works to create geochemical barriers based on other local clays are planned. Remediation and increasing the fertility of soils contaminated with heavy metals are necessary for the prevention of further penetration of these metals into agricultural crops.

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