UDC 681.5.015
DOI: 10.15587/1729-4061.2022.270519

PRINCIPLES AND STAGES OF CREATION OF AUTOMATIC CONTROL SYSTEMS WITH A MODEL OF COMPLEX TECHNOLOGICAL PROCESSES

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The object of this study is an effective approach to designing automatic control systems with a model of complex technological processes, which include interrelated and complementary stages from the formulation of the task to the implementation of the control system at the facility. It includes a set of measures, starting with the analysis of the process in its hardware design with the construction of an information and logical scheme to the development of all types of security and commissioning.

The main problem in the implementation of a control system with a technological process model is the limited ranges of adequacy of mathematical models. Therefore, when changing the load on the unit, changing external and internal perturbations, it is necessary to constantly ensure the necessary level of adequacy of the models. It is proposed to use a combined model as a mathematical model of the control object, combining the advantages of analytical and experimental-statistical models. This makes it possible to significantly expand the information base of the resulting model. A simple and effective iterative algorithm for calculating this model is also proposed. It includes sequential steps to determine the parameters of the model by basic dependences (the deterministic part of the model), followed by clarifying them according to the current data from the object (experimental statistical part of the model). The effectiveness of the approach is confirmed by the example of ASC TP of the ammonia synthesis column. By improving the accuracy of determining the control parameters and narrowing the range of their change around the optimal value, the volume of ammonia release increases by 5–8 %.

The application of the described approach on the example of the development of an automatic control system for the technological process of ammonia synthesis confirmed the economic feasibility of implementing the proposed solutions

Keywords: control system, control with model, information-logical scheme, combined mathematical model, algorithm, optimization

Received date 21.09.2022
Accepted date 09.12.2022
Published date 30.12.2022

How to Cite: *Loriia, M., Tselishchev, O., Eliseyev, P., Porkuian, O., Hurin, O., Abramova, A., Boichenko, S. (2022). Principles and stages of creation of automatic control systems with a model of complex technological processes. Eastern-European Journal of Enterprise Technologies, 6 (6 (120)), 20–29. doi: https://doi.org/10.15587/1729-4061.2022.270519*

1. Introduction

Modern chemical and technological processes are characterized by a large number of high-tech equipment with complex and multiple internal connections. Much of these processes are continuous and multi-tonnage with a large amount of energy and raw materials consumed. Despite the study of existing technological processes and schemes, they have an unrealized technological reserve. It can be used by supporting the technological process under optimal conditions of the required volume of production with minimal consumption of raw materials and energy under any loads and any disturbances. It is impossible to solve such a complex problem using typical automation solutions and relying only on the experience of technological personnel. However, the use of control systems with a model of technological processes allows one to solve such a problem. Despite the large number of works in this area, a unified approach with the established principles for the creation of such systems has not yet been proposed.

Ammonia production is a source of synthetic ammonia. Ammonia is a raw material for the production of nitrate acid, ammonium nitrate, urea, and other chemical products containing nitrogen, and is also used in medicine, in agriculture as a fertilizer, etc. That is why reducing the cost of ammonia will reduce the cost of a number of its derivatives, and therefore increase their competitiveness. The cost of raw materials in recent years in the world has been constantly growing, which negatively affects the competitiveness of Ukrainian industries, which are characterized by high consumption of natural gas in the production of ammonia in particular. It is necessary to solve the issues of more efficient use of raw materials, energy resources, to carry out work on the reconstruction and modernization of production. To do this, it is necessary to increase the efficiency of technological processes, including control systems. This problem is solved by reducing energy and resource consumption. Positive results can be obtained either by improving the existing one or by developing a new management system.

At the same time, ammonia production is complex in technological, hardware, and circuit solutions. It is characterized by extremely high values of technological parameters (temperature, pressure of reaction media), a large number and interconnectivity of parameters. Therefore, when developing a mathematical model, it is necessary to solve the non-trivial task of ensuring its adequacy with maximum simplicity for effective implementation in control systems. At the same time, it should be understood that the functioning of the real technological process is associated with a change in its parameters in a wide range. Therefore, enabling the accuracy of the mathematical model of the process and its adequacy is a separate complex task.

It should be understood that no mathematical model of a physical system is absolutely accurate. It is possible to increase the accuracy of the model, increasing the number and complexity of equations. But at the same time, the form of solving high-order equations will also depend on the values of the coefficients of the model. This, on the one hand, makes it impossible to use algorithms that will work automatically, and on the other hand, it requires the use of approximate solution methods, which significantly reduces the accuracy of the resulting solution. That is, the model must be both one that adequately reflects the behavior of the physical system, and quite simple. Therefore, research into this area is relevant.

2. Literature review and problem statement

Maintaining the technological process under optimal conditions with minimal consumption of raw materials and energy under any loads and disturbances is a difficult task, which is impossible to solve only with a typical approach to automation.

In [1], it is shown that adaptive systems make it possible to accumulate and process information about the behavior of an object in real time. This feature makes it possible to reduce the shortcomings of the lack of information about the system during its design, but in systems with extremely high values of technological parameters (temperature, pressure of reaction media), a large number and interconnectivity of parameters do not solve the problem of optimal control.

In [2], it is shown that the collection of information from standard sources in production does not always fully meet the requirements of the development and design of modern automation systems. In this case, it is advisable to apply the collection and processing of expert information. Experts involve specialists with significant practical experience and knowledge of the studied technological process. But it is impossible to solve a complex problem based only on the experience of technological personnel.

Paper [3] proved the effectiveness of using models of the second-fourth power for the development of mathematical models of technological control objects in order to use these models in automatic control systems. But these models retain adequacy in fairly narrow load ranges on the synthesis column and constantly need to be adjusted by recalculating the coefficients of the model.

In [4], it is shown that the parameters of a complex object, synthesis column, have complex and multiple internal connections. Therefore, a change in the flow rate of synthesis gas through any of the cold bypasses leads not only to a change in temperature on the corresponding shelf but also to a change in all costs through the physical channels of the column. That is, by changing the flow rate of synthesis gas in the pipeline of any of the cold bypasses of the column, the entire temperature regime of the column will change, and, as a result, the concentration of the target component at the outlet of the column.

In [5], it is shown that in order to achieve the maximum possible production efficiency, synthesis gas costs should be distributed in this way through the physical channels of the synthesis column so that the concentration of the target component at the outlet of the column is maximum. At the same time, the temperature on the shelves of the methanol synthesis column should not exceed the permissible value. But the problem of creating a mathematical model and tracking the current state of the control object and constantly comparing the initial coordinates of the process, calculated according to the object model, with their current values, is not considered.

The statement of the features of the technological process has found its justification and in-depth analysis in work [6]. It is shown that the impossibility of directly solving the problem is associated with the fundamental features of the object, namely the abundance of technological parameters, the change of each of which will shift the extremum of concentration. But the approach to the solution and measures to improve the efficiency of work to the creation of optimal control systems with the model is not considered.

In [7], the issue of developing a mathematical model of a technological object is considered but the fact that in order to create a mathematical model of a complex process, it is necessary to solve the non-trivial problem of ensuring its adequacy at maximum simplicity for effective implementation in the control system was not considered. Because the functioning of the real technological process is associated with a change in its parameters in a wide range. Therefore, ensuring the accuracy of the mathematical model of the process and its adequacy is a separate complex task.

This approach is used in [8]. However, the model of ideal pushing out with a gradient of parameters along the spatial coordinate was chosen as a model. The use of such a model is impossible because of the complexity of identifying the parameters of the model. An option to overcome this problem is to use a control system with a model.

Analysis of [9], which considers the development of a static and dynamic model of the shelves of the synthesis column and the internal heat exchanger, confirms the conclusions drawn. But the issue of creating a control system for a technological object has not been considered.

In [10], the algorithm of functioning of the control system with a model is proposed. But the ways of implementation and configuration of control systems with a model are not indicated because when developing a control system with a model of an ammonia synthesis column in ammonia production, the question of the possibility of practical implementation of the proposed solutions is important.

Taking into account the analysis, we can say that the use of a technological resource to optimize production in full requires a unified approach to the creation of control systems for complex processes, which includes interrelated and complementary stages from setting a task to implementing a control system at the facility. It includes a set of measures, starting with the analysis of the process in its hardware design with the construction of an information and logical scheme to the development of all types of security and practical implementation.

3. The aim and objectives of the study

The purpose of this work is to develop an approach to the management of complex technological processes with a model, including an algorithm for functioning on the example of a synthesis column in ammonia production. This will make it possible to narrow the range of parameters of the technological process around the optimal value, which will lead to a real economic effect.

To accomplish the aim, the following tasks have been set:

– to analyze the processes in a three-field reactor (column) of ammonia synthesis with a built-in heat exchanger;

– to build appropriate information and logical schemes;

– to develop direct and inverse mathematical models of ammonia synthesis column and heat exchanger;

– based on the analysis of the information-logical scheme of a three-field gas reactor with a built-in heat exchanger, to develop an algorithm for the functioning of the control system with a model;

– to propose the practical implementation of the proposed algorithm;

4. The study materials and methods

Based on the generalization of many years of experience in the development of automation systems, the authors propose a unified approach and measures to improve the efficiency of work to the creation of optimal control systems with a model of complex technological processes.

The basis of such systems is the study of the current state of the control object and the constant comparison of the initial coordinates of the process, calculated according to the object model, with their current values. This will make it possible to constantly monitor the adequacy of the mathematical model of the object and, in the event of significant deviations between the measured and calculated values, signal the need to adjust the mathematical model.

As an example of the application of the proposed approach, ammonia production was chosen. The principle of development of control systems with a model of technological process was proposed. Structurally, the principle of creating a control system with a model of complex technological processes is shown in Fig. 1.

The principle covers all stages of building a control system with a technological process model, the implementation of which requires a significant amount of work. In this paper, the authors focused on the development of some of them, formulating the methodological foundations for creating control systems with a model of complex technological processes.

At the first stage, it is necessary to analyze the technological process as a control object.

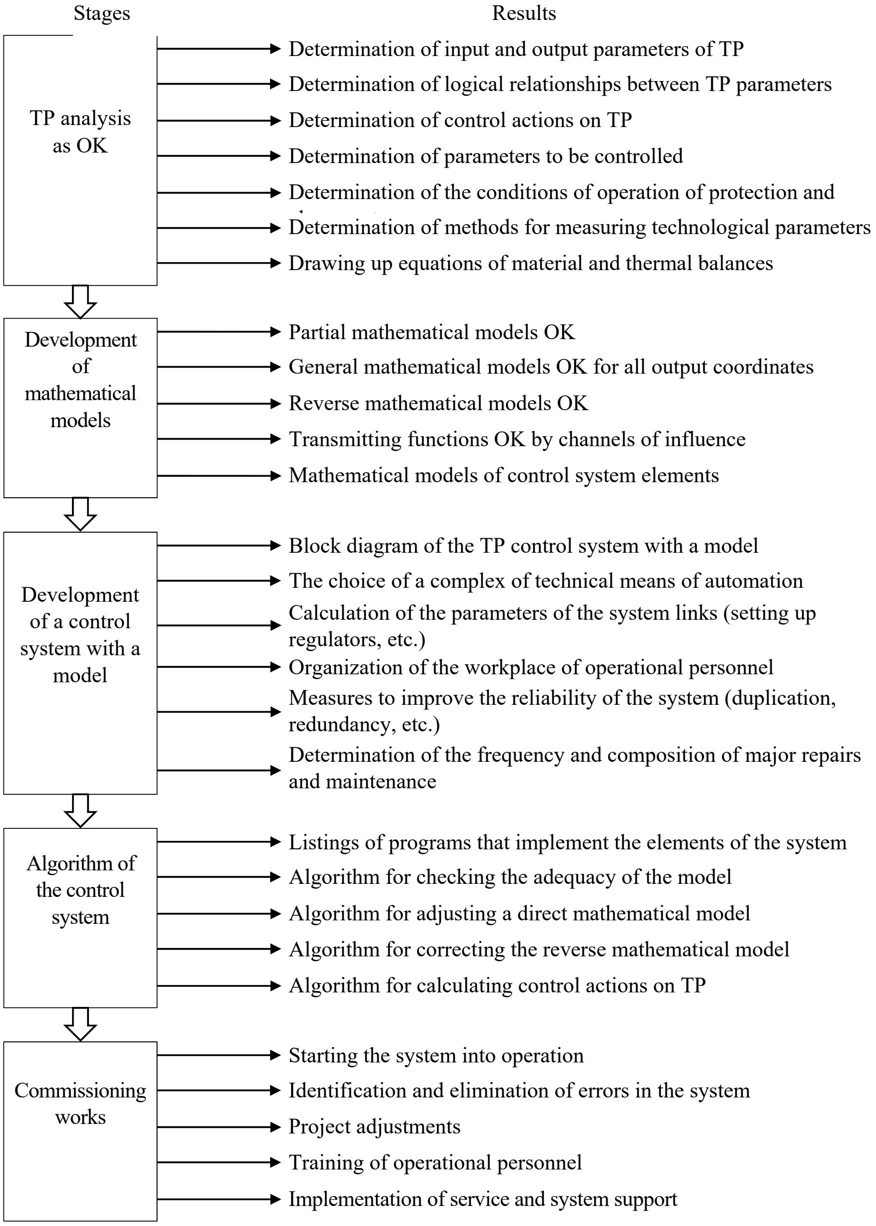

Fig. 1. The principle of creating a control system with a model of complex technological processes

To develop a control system for a complex technological process, it is necessary to perform an analysis of the technological process as a control object. To do this, an analysis of information transformations accompanying technological transformations is made.

5. Results of development and research of the mathematical model of the ammonia synthesis column in ammonia production

5. 1. Analysis of processes in a three-field reactor

The task of this stage of system development is to determine the input and output coordinates of the process and establish logical connections between them, determine the control actions. It is also necessary to determine the parameters to be controlled, determine the conditions for triggering protection and signaling systems, determine the methods for measuring technological parameters, and draw up equations for material and thermal balances.

Data for analysis can be obtained from technical literature, technological regulations, operator logs or databases of values of controlled parameters, etc.

But practice shows that the collection of information from standard sources in production does not always fully meet the requirements of the development and design of modern automation systems. In this case, it is advisable to apply the collection and processing of expert information [1]. Experts involve specialists with significant practical experience and knowledge of the studied technological process. The use of expert data can significantly reduce the amount of experimental research, as well as the need for statistical data on production.

For parameters, whose technological relationship is not obvious (for example, fixed in technological regulations), if possible, additional research should be carried out and data for correlation analysis should be collected. Such parameters are likely to be perturbation parameters and will be probabilistic in nature.

If we consider the technological process as a connected information network that implements causal relationships of parameters, then it is convenient to arrange the analysis of this process in the form of a graphic information and logical scheme [2].

When carrying out the process of ammonia synthesis in the production of ammonia, it is necessary to ensure the maximum degree of conversion of the nitrogen-hydrogen mixture into ammonia in the reversible synthesis reaction by maintaining the optimum temperature along the height of the synthesis column. The temperature on the shelves of the column is regulated by changing the flow rate of the nitrogen-hydrogen mixture through the channels of «cold» bypasses on each shelf of the column. The mathematical model of the ammonia synthesis column is a system of equations, which includes mathematical models of the shelves of the column synthesis and mathematical model of the heat exchanger. At the same time, the algorithm of the model, for example, for the first shelf of the column, is similar for both the second and third shelves. The information-logical scheme of the shelf of the ammonia synthesis column is shown in Fig. 2.

The output parameters (coordinates) of the process are the concentration Q of ammonia at the outlet of the reactor shelf, the temperature T at the outlet of the reactor shelf, and the pressure P. In the production of ammonia, pressure P is determined by the operation of the compressor, that is, it is a disturbing parameter. When controlling gas reactors, only temperature is regulated, and the concentration is only controlled.

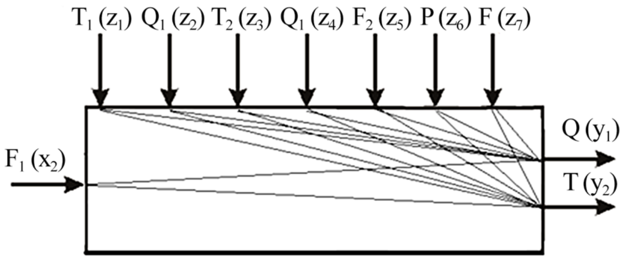

Fig. 2. Information-logical scheme of the shelf of a gas reactor

The input parameter of the process is the gas flow through the "cold" bypass F_1. The flow rate of the gas mixture along the main course at the inlet of column F_2 and at the inlet of each shelf cannot be adjusted, so it is referred to as perturbations.

Also, disturbing coordinates are the temperatures of the input streams T_1 and T_2 and the concentration Q_1 and Q_2 in their target component.

All coordinates at the output will change if at least one input parameter or disturbing coordinate changes. That is, they are interconnected.

To obtain a complete MM column for ammonia synthesis, it is also necessary to develop a MM for a shell-and-tube heat exchanger. The process of obtaining a mathematical model of a heat exchanger is standard.

The information-logical scheme of the remote shell-and-tube heat exchanger is shown in Fig. 3.

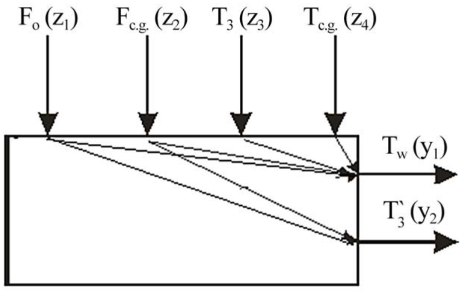

Fig. 3. Information-logical scheme of remote shell-and-tube heat exchanger

For the internal heat exchanger of the column, the output coordinates are the temperature of the circulating gas at the outlet of the heat exchanger T_3' and the wall temperature through which heat transfer T_w is carried out. There are no input regulatory coordinates because there are no costs that could be changed at the input of the templo-exchanger. The remaining coordinates: synthesis gas flow rate along the main cours F_0, $F_{c.g.}$, the temperature of the circulating gas at the outlet of the third shelf (at the inlet of the heat exchanger) T_3 and $T_{c.g.}$, the temperature of the gas along the main course, shown in Fig. 3, should be attributed to the disturbing parameters.

The task is to develop a methodology for creating effective control systems with a model of complex technological processes. The system was based on the study of the current state of the control object. This will make it possible to constantly monitor the adequacy of the mathematical model of the object and, in the event of significant deviations between the measured and calculated values, signal the need to adjust the mathematical model.

This analysis shows that in order to obtain a general mathematical model of the ammonia synthesis column, it is necessary to compile models of three shelves of the column and the internal heat exchanger.

Technological audit of ammonia production allows us to conclude that the technological resource of the scheme is not fully used. It can be increased by maintaining the optimal mode of operation of the ammonia synthesis column at all possible loads and permissible values of disturbing parameters. In addition, when developing a control system with a model of an ammonia synthesis column in ammonia production, it is important to resolve the issue of the possibility of practical implementation of the proposed solutions without losing the level of economic feasibility that needs to be achieved.

5. 2. Creation of information and logical schemes

A generalized information-logical scheme of the ammonia synthesis column with the built-in internal heat exchanger was compiled. Schematically, a three-shelf ammonia synthesis column with a built-in internal heat exchanger can be given in the form of Fig. 4.

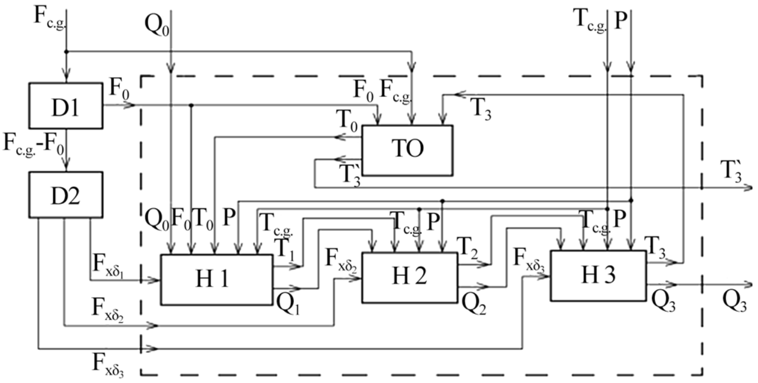

Fig. 4. Information-logical scheme of a three-field gas reactor with a built-in heat exchanger

In Fig. 4, H1, H2, H3 are the shelves of the synthesis column, TO – internal heat exchanger, D1, D2 – mathematical flow division operators

Thus, as a result of the analysis of the technological process occurring in the ammonia synthesis column, the input regulating, input disturbing, and output coordinates of this process were determined, and a logical connection between them was established. This analysis shows that in order to obtain a general mathematical model of the ammonia synthesis column, it is necessary to compile models of three shelves of the column and the internal heat exchanger.

5. 3. Development of direct and inverse mathematical models of ammonia synthesis column and heat exchanger

The algorithm for determining the mathematical model of the ammonia synthesis column is similar to the assembly of MM for an ammonia synthesis column [3]. To determine the MM of the column, it is necessary to make two partial models: by the concentration Q of the target component (ammonia) and by the temperature T.

The equation of material balance for the target component takes the form.

$$dm_1 + dm_2 + dm_p = dm_v + dm, \quad (1)$$

where dm_1 is the mass of ammonia that enters the reactor with the first flow;

dm_2 – mass of ammonia that enters the reactor with a second flow;

dm_p – mass of ammonia, which is formed in the reaction;

dm_v – mass of ammonia that accumulates in the reactor with volume V;

dm – the mass of ammonia that is discharged from the reactor.

The equation in technological variables is:

$$dm_1 = F_1 Q_1\, dt, \quad (2)$$

where F_1 is the consumption of nitrogen-hydrogen mixture along the "main" course at the entrance of the shelf, kg/s;

Q_1 – concentration of ammonia in the flow of the "main" course, mass fraction;

dt – time increase, s.

$$dm_2 = F_2 Q_2\, dt, \quad (3)$$

where F_2 is the consumption of nitrogen-hydrogen mixture by "cold" bypass at the entrance of the shelf, kg/s;

Q_2 – concentration of ammonia in the "cold" bypass, mass fraction;

$$dm_p = \rho V K \left(Q - Q_p\right) dt, \quad (4)$$

where ρ is the density of nitrogen-hydrogen mixture in the reactor (determined from the Mendeleev-Clapeyron equation), kg/m^3;

V – reaction volume of the gas reactor, m^3;

K – chemical reaction rate, 1/s;

Q and Q_p – ammonia concentration at the outlet and at the reactor shelf inlet, respectively.

In the case of the first shelf, the concentration of ammonia in the flow of the "main" flow and the "cold" bypass Q_1 and Q_2 are equal, and, in the calculation, they can be equated to the value of Q_n. In the case of the second and third shelves, the concentration of ammonia Q_n is obtained by mixing two streams and, accordingly, will be determined by the formula:

$$Q_n = \frac{F_1 Q_1 + F_2 Q_2}{F_1 F_2}. \quad (5)$$

The dependence of the rate of chemical reaction K on the process temperature is determined by the Arrhenius equation

$$K = K_0 \exp\left(-\frac{E}{RT}\right), \quad (6)$$

where K_0 is the reaction rate constant, 1/s;

E – reaction activation energy, J/mol;

R – universal gas constant, J/(mol K);

T – reaction temperature, K.

$$dm_V = \rho V dQ, \quad (7)$$

where ρ is the density of the gas mixture of the reactor, kg/m^3;

V – free volume of the reactor, m^3;

dQ – change in the concentration of ammonia in the reactor, mass fraction.

$$dm = FQ\, dt, \quad (8)$$

where F is the gas mixture consumption at the outlet of the reactor shelf, kg/s;

Q – concentration of ammonia at the reactor outlet, mass fraction.

In technological variables, the equation takes the form:

$$F_1Q_1\,dt+F_2Q_2\,dt+\rho VK_0\exp\left(-\frac{E}{RT}\right)\times$$
$$\times\left(Q-\frac{F_1Q_1+F_2Q_2}{F_1+F_2}\right)dt==\rho VdQ+\left(F_1+F_2\right)Qdt. \tag{9}$$

After the necessary mathematical transformations (the method of obtaining mathematical models is set out in [4]), we obtain a partial model of the shelf of the ammonia synthesis column in ammonia production (excluding the delay time) in canonical form.

$$\tau_1\frac{dy_1}{dt}+y_1=K_{11}x_1+K_{12}z_1+$$
$$+K_{13}z_3+K_{14}z_4+K_{15}z_5+K_{16}y_2. \tag{10}$$

In equation (10), the designations of dimensionless coordinates correspond to the notation adopted in Fig. 2. K_{11}, ..., K_{16} are dimensionless coefficients, and τ_1 is the time constant measured in seconds.

In order to develop a partial mathematical model of the shelf of the ammonia synthesis column by temperature, it is necessary to make an equation for the thermal balance of the shelf (reactor). Heat enters the reactor with two streams of incoming reagents and is released during the synthesis of ammonia. This heat accumulates in the volume of the shelf (heat accumulates in the volume of the catalyst and in the volume of the nitrogen-hydrogen mixture on the shelf) and leaves the shelf with a flow rate equal to the sum of the input costs. The general equation of heat balance is:

$$dq_1+dq_2+dq_p=dq_V+dq, \tag{11}$$

where dq_1 is the amount of heat that comes with the first flow;

dq_2 – the amount of heat that comes with the second stream;

dq_p – the amount of heat that is released as a result of the reaction;

dq_v – the amount of heat that accumulates in the volume of the shelf;

dq – the amount of heat that comes out with the output flow.

We write the heat balance equation in technological variables:

$$dq_1=F_1c_1T_1dt, \tag{12}$$

where F_1 is the consumption of nitrogen-hydrogen mixture on the main course, kg/s;

c_1 – heat capacity of nitrogen-hydrogen mixture in the main stroke flow, J/(kg K);

T_1 – the flow temperature of the main course at the entrance of the shelf, K:

$$dq_2=F_2c_2T_2dt, \tag{13}$$

where F_2 is the consumption of nitrogen-hydrogen mixture by "cold" bypass, kg/s;

c_2 – heat capacity of the flow supplied by the "cold" bypass, J/(kg K);

T_2 – the flow temperature of the "cold" bypass, K.

$$dq_p=r\rho VK\left(Q-Q_n\right)dt, \tag{14}$$

where r is the specific heat of reaction, J/kg;

ρ – density of the gas mixture in the reactor (determined from the Mendeleev–Clapeyron equation), kg/m^3;

V – free volume of the gas reactor, m^3;

K – chemical reaction rate, 1/s;

Q and Q_n is the concentration of ammonia at the outlet and at the inlet to the reactor, respectively, mass fraction.

$$dq_V=\rho VcdT, \tag{15}$$

where ρ is the density of the gas mixture in the reactor (determined from the Mendeleev–Clapeyron equation), kg/m^3;

V – free volume of the reactor, m^3;

c – heat capacity of the gas mixture in the reactor, J/(kg K);

dT – temperature change in the reactor, K.

$$dq=FcT\,dt, \tag{16}$$

where F is the gas consumption from the reactor (determined by the sum of the costs F_1 and F_2, kg/s;

c – heat capacity of the gas mixture that comes out of the reactor, J/(kg K);

T – temperature in the reactor, K.

Taking into account the above, the heat balance equation in technological variables will take the form

$$F_1c_1T_1dt+F_2c_2T_2dt+$$
$$+\frac{rPV}{RT}K_0\exp\left(-\frac{E}{RT}\right)\left(Q-\frac{F_1Q_1+F_2Q_2}{F_1+F_2}\right)dt=$$
$$=\frac{PVc}{RT}dT+\left(F_1+F_2\right)cTdt. \tag{17}$$

After all the transformations, the model will take the following form:

$$\tau_2\frac{dy_2}{dt}+y_2=K_{21}x_1+K_{22}z_1+K_{23}z_2+$$
$$+K_{24}z_3+K_{25}z_4+K_{26}z_5+K_{27}z_6+K_{28}y_1, \tag{18}$$

where τ_2 is the time constant, s; K_{21}; K_{22} – coefficients of the model.

Thus, we have a system:

$$\begin{cases}\tau_1\dfrac{dy_1}{dt}+y_1=K_{11}x_1+K_{12}z_1+\\+K_{13}z_3+K_{14}z_4+K_{15}z_5+K_{16}y_2,\\\tau_2\dfrac{dy_2}{dt}+y_2=K_{21}x_1+K_{22}z_1+K_{23}z_2+\\+K_{24}z_3+K_{25}z_4+K_{26}z_5+K_{27}z_6+K_{28}y_1.\end{cases} \tag{19}$$

The solution of the system of equations with respect to y_1 is a dynamic mathematical model of the shelf of the synthesis column by concentration, and to y_2 – a dynamic mathematical model by temperature.

The dynamic mathematical model of the shelf of the ammonia synthesis column by ammonia concentration is:

$$\begin{aligned}&T_{11}^2\frac{d^2y_1}{dt^2}+T_{12}\frac{dy_1}{dt}+y_1=\\&=K_{31}\left(T_{13}\frac{dx_1}{dt}+x_1\right)+K_{32}\left(T_{14}\frac{dz_1}{dt}+z_1\right)+\\&+K_{33}z_2+K_{34}\left(T_{15}\frac{dz_3}{dt}+z_3\right)+\\&+K_{35}\left(T_{16}\frac{dz_4}{dt}+z_4\right)+K_{36}\left(T_{17}\frac{dz_5}{dt}+z_5\right)+K_{37}z_6.\end{aligned}\tag{20}$$

where

$$H_3=\frac{1-K_{28}K_{16}}{K_{16}};\quad K_{31}=\frac{K_{11}+K_{21}}{1-K_{28}K_6};$$

$$K_{32}=\frac{K_{12}+K_{22}}{1-K_{28}K_6};\quad K_{33}=\frac{K_{23}}{H_3};$$

$$K_{34}=\frac{K_{13}+K_{24}}{1-K_{28}K_6};\quad K_{35}=\frac{K_{14}+K_{25}}{1-K_{28}K_6};$$

$$K_{36}=\frac{K_{15}+K_{26}}{1-K_{28}K_6};\quad K_{37}=\frac{K_{23}}{H_3};$$

– coefficients

$$T_{11}^2=\frac{\tau_1\tau_2}{H_3K_{16}};\quad T_{12}=\frac{\tau_1+\tau_2}{H_3K_{16}};\quad T_{13}=\frac{\tau_2K_{11}}{H_3\left(K_{11}+K_{21}\right)};$$

$$T_{14}=\frac{\tau_2K_{12}}{H_3\left(K_{12}+K_{22}\right)};\quad T_{15}=\frac{\tau_2K_{13}}{H_3\left(K_{13}+K_{23}\right)};$$

$$T_{16}=\frac{\tau_2K_{14}}{H_3\left(K_{14}+K_{25}\right)};\quad T_{17}=\frac{\tau_2K_{15}}{H_3\left(K_{15}+K_{26}\right)};$$

– time constants.

Dynamic MM for temperature on the first shelf of the ammonia synthesis column takes the form:

$$\begin{aligned}&T_{21}^2\frac{d^2y_2}{dt^2}+T_{22}\frac{dy_2}{dt}+y_2=K_{41}\left(T_{23}\frac{dx_1}{dt}+x_1\right)+\\&+K_{42}\left(T_{24}\frac{dz_1}{dt}+z_1\right)+K_{43}\left(T_{25}\frac{dz_2}{dt}+z_2\right)+\\&+K_{44}\left(T_{26}\frac{dz_3}{dt}+z_3\right)+K_{45}\left(T_{27}\frac{dz_4}{dt}+z_4\right)+\\&+K_{46}\left(T_{28}\frac{dz_5}{dt}+z_5\right),\end{aligned}\tag{21}$$

where

$$H_4=\frac{1+K_{16}K_{28}}{K_{28}};\quad K_{42}=\frac{K_{12}K_{28}+K_{22}}{H_4K_{28}};$$

$$K_{43}=\frac{K_{23}}{H_4K_{28}};\quad K_{44}=\frac{K_{13}K_{28}+K_{24}}{H_4K_{28}};$$

$$K_{45}=\frac{K_{14}K_{28}+K_{25}}{H_4K_{28}};\quad K_{46}=\frac{K_{15}K_{28}+K_{26}}{H_4K_{28}};$$

– coefficients.

$$T_{21}^2=\frac{\tau_1\tau_2}{H_4K_{28}};\quad T_{22}=\frac{\tau_1+\tau_2}{H_4K_{28}};$$

$$T_{23}=\frac{\tau_1K_{21}}{H_4\left(K_{28}K_{11}+K_{21}\right)};\quad T_{24}=\frac{\tau_2K_{12}}{H_4\left(K_{12}K_{28}+K_{22}\right)};$$

$$T_{25}=\tau_1;\quad T_{26}=\frac{\tau_1K_{24}}{H_3\left(K_{13}K_{28}+K_{24}\right)};$$

$$T_{27}=\frac{\tau_1K_{25}}{H_4\left(K_{14}K_{28}+K_{25}\right)};\quad T_{28}=\frac{\tau_1K_{26}}{H_4\left(K_{15}K_{28}+K_{26}\right)}.$$

The system of equations (21) is a static MM of the first shelf of the ammonia synthesis column in ammonia production. Solving this system of equations with respect to the concentration of ammonia at the output of the shelf of the synthesis column or with respect to the temperature of the nitrogen-hydrogen mixture at the output of the shelf, we obtain an equation that connects this output parameter with all the input parameters of the process.

$$\begin{cases}F_{10}Q_{10}+F_{20}Q_{20}+\rho VK_0\exp\left(-\dfrac{E}{RT_0}\right)\times\\ \times\left(Q_0-\dfrac{F_{10}Q_{10}+F_{20}Q_{20}}{F_{10}+F_{20}}\right)=\left(F_{10}+F_{20}\right)Q_0,\\ F_{10}c_1T_{10}+F_{20}c_2T_{20}+\dfrac{rP_0V}{RT_0}K_0\exp\left(-\dfrac{E}{RT_0}\right)\times\\ \times\left(Q_0-\dfrac{F_{10}Q_{10}+F_{20}Q_{20}}{F_{10}+F_{20}}\right)=\left(F_{10}+F_{20}\right)cT_0.\end{cases}\tag{22}$$

The difference between obtaining MM of the second and third shelves of the synthesis column is entirely that the output flow from the first shelf is the input flow of the main course for the second shelf. The flow that comes out of the second shelf is for the third. At the same time, the parameters of cold bypass fed to the second and third shelves will be the same.

Static MMs of the second and third shelves of the ammonia synthesis column take the following form:

$$\begin{cases}F_{10}Q_{10}+F_{20}Q_{20}+\rho VK_0\exp\left(-\dfrac{E}{RT_0}\right)\times\\ \times\left(Q_0-\dfrac{F_{10}Q_{10}+F_{20}Q_{20}}{F_{10}+F_{20}}\right)=\left(F_{10}+F_{20}\right)Q_0,\\ F_{10}c_1T_{10}+F_{20}c_2T_{20}+\dfrac{rP_0V}{RT_0}K_0\exp\left(-\dfrac{E}{RT_0}\right)\times\\ \times\left(Q_0-\dfrac{F_{10}Q_{10}+F_{20}Q_{20}}{F_{10}+F_{20}}\right)=\left(F_{10}+F_{20}\right)cT_0,\end{cases}\tag{23}$$

$$\begin{cases}F_{10}Q_{10}+F_{20}Q_{20}+\rho VK_0\exp\left(-\dfrac{E}{RT_0}\right)\times\\ \times\left(Q_0-\dfrac{F_{10}Q_{10}+F_{20}Q_{20}}{F_{10}+F_{20}}\right)=\left(F_{10}+F_{20}\right)Q_0,\\ F_{10}c_1T_{10}+F_{20}c_2T_{20}+\dfrac{rP_0V}{RT_0}K_0\exp\left(-\dfrac{E}{RT_0}\right)\times\\ \times\left(Q_0-\dfrac{F_{10}Q_{10}+F_{20}Q_{20}}{F_{10}+F_{20}}\right)=\left(F_{10}+F_{20}\right)cT_0.\end{cases}\tag{24}$$

Equation (25) is a dynamic MM for an internal heat exchanger of an ammonia synthesis column in ammonia production.

$$T_2^2\frac{d^2y_1}{dt^2}+T_1\frac{dy_1}{dt}+y_1=K_{31}x_1+K_{32}\left(T_{31}\frac{dz_1}{dt}+z_1\right)+$$
$$+K_{33}\left(T_{32}\frac{dz_2}{dt}+z_2\right)+K_{34}z_3, \qquad (24)$$

where $T_2^2=\frac{\tau_1\tau_2}{1-K_{13}K_{23}}$ – time constant, s^2;

$T_1=\frac{\tau_1+\tau_2}{1-K_{13}K_{23}}$; $T_{31}=T_{32}=\tau_1$ – time constants, s;

$H_3=\frac{1-K_{13}K_{23}}{K_{23}}$; $K_{31}=\frac{K_{11}K_{23}}{1-K_{13}K_{23}}$;

$K_{32}=\frac{K_{21}}{1-K_{13}K_{23}}$; $K_{33}=\frac{K_{22}}{1-K_{13}K_{23}}$;

$K_{34}=\frac{K_{12}}{1-K_{13}K_{23}}$ – model's coefficients.

A system of equations (25) is a system of equations that is a static MM for an internal heat exchanger of an ammonia synthesis column.

$$\begin{cases}F_{T0}c_TT_{T_{10}}=\alpha_2S_2\left(T_{cm0}-T_{n0}\right)+F_{T0}c_TT_{T_{20}},\\ F_{n0}c_nT_{n_{10}}+\alpha_2S_2\left(T_{cm0}-T_{n0}\right)=F_{n0}c_nT_{n_{20}}.\end{cases} \qquad (25)$$

Systems of equations (22) to (24) and (25) make up a system of static models of the ammonia synthesis column. The solution of this system of equations with respect to the concentration of ammonia at the output of the third shelf of the column (at the output of the column) is actually the reverse mathematical model of the ammonia synthesis column. It can be given as follows.

$$a_4Q_3^4+a_3Q_3^3+a_2Q_3^2+a_1Q_3+a_0=$$
$$=\varphi_1\left(F_{cb1}\right)+\varphi_2\left(F_{cb2}\right)+\varphi_3\left(F_{cb3}\right)+$$
$$+\varphi_{12}\left(F_{cb1},F_{cb2}\right)+\varphi_{13}\left(F_{cb1},F_{cb2}\right)+$$
$$+\varphi_{23}\left(F_{cb2},F_{cb3}\right)+{}^{\backprime}\Omega\left(F_{cb1}F_{cb2}F_{cb3}\right)+$$
$$+{}^{\backprime}\Omega\left(F_{cg},T_{cg},Q\right), \qquad (26)$$

where a_4, a_3, a_2,a_1, a_0 are the coefficients of the model;

Q – concentration of ammonia at the outlet of the column;

F_{cg}, F_{cb1}, F_{cb2}, F_{cb3} – synthesis gas consumption over all input flows of the reactor (main course and "cold" bypasses);

T_{cg}, Q_0, P – temperature, concentration of the target component, and pressure of the circulating gas;

${}^{\backprime}\Omega\left(F_{cg},T_{cg},Q\right)$ – functionality of the influence of disturbing parameters;

φ_1, φ_2, φ_3, φ_{12}, φ_{23}, φ_{13}, φ_{123} – functions that take into account the effect of changes in costs on changes in ammonia concentration at the outlet of the column.

Equation (26) is a mathematical model of a three-shelf ammonia synthesis column. The deterministic approach allowed for structural identification and determination of the type of mathematical model of the ammonia synthesis column in ammonia production. As a model, the fourth-order equation for the concentration of ammonia is adopted. This model is the starting point for a control system with a methanol synthesis column model in methanol production. The model is quite simple: in a fourth-order equation, an unknown quantity can always be determined through the coefficients of the equation. That is, when adapting the model, the functional appearance of dependences will not change, and only the coefficients will change.

The solution of this equation can be used as a criterion equation to solve the optimization problem. In general, it can be written as follows

$$Q_3=f\left(F_{cg},F_{cb1},F_{cb2},F_{cb3},T_{cg},Q_0,P\ldots\right). \qquad (27)$$

Thus, in the proposed technique for creating automatic control systems with a model of complex technological objects, direct and reverse mathematical models can be obtained.

5. 4. Development of an algorithm for the functioning of the control system with a model

The main tasks of this stage are listing programs that implement the elements of the system; development of algorithms for checking the adequacy of mathematical models; development of algorithms for correcting direct and reverse mathematical models; development of an algorithm for calculating the optimal control effects.

The main problem in the implementation of a control system with a technological process model is the limited ranges of adequacy of mathematical models. Therefore, when changing the load on the unit, changing external and internal perturbations, it is necessary to constantly check the adequacy of the obtained models. If the deviation between the measured and modeled process parameters exceeds the established limit, the mathematical model should be adjusted. It is proposed to do this as follows. If a situation arises in which the model ceases to be adequate, the left side of equation (27) is equated to the measured value. Using the least squares method, we calculate the values of the coefficients of the left side of the equation. After that, the coefficients of the right side of the equation are recalculated. If the adjusted mathematical model becomes adequate again, the coefficients of the reverse model are recalculated. Thus, in the proposed method of creating control systems with a model of complex technological processes, it is proposed to carry out the procedure for maintaining the adequacy of the mathematical model.

To search for the extreme of the criterion equation (27) of the dependence of the ammonia concentration at the output of the column on the values of synthesis gas consumption by cold bypasses, an algorithm based on the Hook-Jives method is proposed on the first or third shelf of the column.

5. 5. Development of a control system with a model

The main tasks of this stage are the development of a block diagram of the control system with a model, the choice of a set of technical means, the calculation of the parameters of the system links; organization of the workplace of operational personnel. It is also necessary to develop measures to improve the reliability of the system, determine the frequency and composition of major repairs and maintenance.

Schematically, the control system with the model of the ammonia synthesis column in ammonia production, which implements the strategy of optimal control over the ammonia synthesis column, is shown in Fig. 5.

Commissioning works.

The last stage of creating a control system with a model of complex technological processes is commissioning. It includes installation of the system; starting the system into operation; project adjustment; training of operational personnel; implementation of service maintenance and system support. As a rule, this stage is implemented by special organizations.

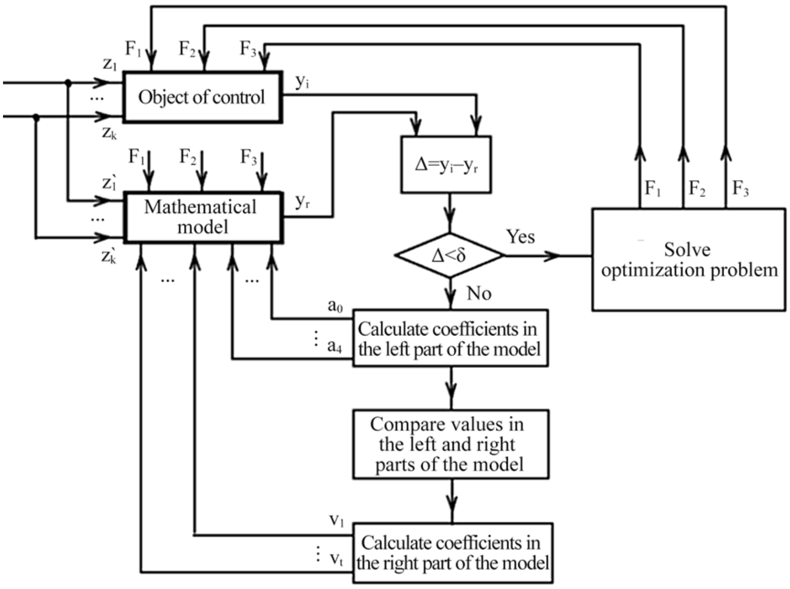

Fig. 5. Block diagram of the algorithm for the functioning of the control system with a model

6. Discussion of results of the study of the control system with the model of the ammonia synthesis column in ammonia production

Thus, using the proposed method of developing control systems with a model of complex technological processes, a control system with a model of ammonia synthesis column in ammonia production was developed as an example. The proposed system works as follows. The cost values of “cold” bypasses, the “main” course, as well as all other parameters of the column, which are included in the model by the concentration of the ammonia synthesis column, are measured using appropriate information and measuring channels. The values are converted to digital form and fed to the input of the mathematical model of the column by concentration. At the output of the ammonia synthesis column, values of ammonia concentration and gas temperature are formed. These values are also measured by the corresponding information-measuring channels. At the output of the algoblock, which implements the mathematical model of the synthesis column, the calculated values of the ammonia concentration and gas temperature at the outlet of the column are formed (Fig. 5). The calculated value of the ammonia concentration is compared with the real measured value of the ammonia concentration at the output of the column, and the calculated temperature value is compared with the real measured temperature value at the output of the column. If the difference between the measurements and the calculated values at the output of the column of ammonia concentration and gas temperature exceeds a certain specified value, then the model adjustment algorithm starts.

After performing the procedure for adjusting the coefficients of the mathematical model (26), the difference between the measurements and the calculated values of ammonia concentration and gas temperature at the output of the column will not exceed the specified value.

When this condition is met, the procedure for finding the optimal solution is launched. From the revised mathematical model of the ammonia synthesis column by concentration, the optimality criterion is formed. In fact, it is a derivative of the concentration of ammonia at the output of the column for the expenditure of “cold” bypasses, equal to zero. After that, there is the maximum possible concentration of ammonia under these conditions at the outlet of the synthesis column and the corresponding values of the costs of “cold” bypasses. The obtained cost values of “cold” bypasses are listed in the degree of opening of the corresponding valves. These values converted into a control signal are fed to the control valve. When changing the costs of “cold” bypasses and the “main” course in the ammonia synthesis column, there will be a redistribution of internal flows. As a result, transients will begin associated with a change in the temperature profile along the height of the column and, as a result, with a change in the concentration of ammonia at the outlet of each shelf of the column. As the system moves to the new set mode, the process of recalculating the static column model stops. After the cessation of transients in the column, an algorithm for checking the adequacy of a static mathematical model of the technological process and, if necessary, an algorithm for adapting a mathematical model is launched. After adapting the model, an optimization model is solved, when the optimal cost values of “cold” bypasses and the “main” course are determined. The movement to the optimal value will continue until the moment these values coincide with the current ones.

For more accurate configuration of the system, the Hook-Jives algorithm is activated.

The implementation of the algorithm proposed in [10] is quite complex and possible due to the possibility of widespread use of existing powerful computer equipment. Due to the fact that the speed and volume of computational procedures ceases to be a critical limitation of the system, it becomes possible to optimize the structure of the system, improve the friendliness of the interface, as well as the quality and reliability of the system as a whole [8–10].

When developing a control system with a model of an ammonia synthesis column in ammonia production, the question of the possibility of practical implementation of the proposed solutions is important. To ensure the operation of the proposed algorithm, it is necessary to have real values of a number of technological parameters. Among the parameters is the consumption of nitrogen-hydrogen mixture on the synthesis column (load on the column). Other parameters are gas consumption on the «main» course, the cost of «cold» bypasses on the first, second, and third shelves of the column. As well as the concentration of ammonia before the synthesis column and at its outlet, the pressure drop on the column, the pressure in the synthesis cycle, the temperature of the nitrogen-hydrogen mixture in front of the column.

The proposed approach allows, on the basis of solving the optimization problem, obtaining such values of the costs of «cold» bypasses, in which the column will work under conditions close to optimal. This allows you to make a quick «throw» of the system in an area close to optimal. After that, the optimal value of ammonia concentration at the output of the synthesis column (maximum value) in practice is using the Hook-Jives method. A functional automation scheme has been developed and a set of technical means necessary for the implementation of the proposed system is analyzed.

An approach to creating control systems with a model of complex technological processes has been developed. The main stages of the process of creating such systems and the main tasks of each of these stages are determined.

On the example of an ammonia synthesis column in ammonia production, the possibility of applying the proposed methodology for creating a control system with a model is given.

In addition, the paper proposes an approach to the development of a mathematical model for further optimization and control of a complex technological object. At the same time, the combined form of the model allows using the advantages of experimental-statistical and deterministic approaches to achieve high adequacy, easy adaptability, and a wide range of applications, which are key aspects in optimizing and managing complex technological objects. Using this approach, a model of a three-shelf gas reactor (synthesis column) in ammonia production has been developed. Based on the results obtained, programs are developed for the implementation of the proposed algorithms in the automated process control systems for ammonia production, and work is underway to adapt them to ammonia production.

The introduction of this system will narrow the range of parameters of the technological process around the optimal value, which will lead to a real economic effect. Thus, when introducing a control system with a model on a computer imitator for ammonia production, it was possible to increase the concentration of ammonia at the outlet of the column from 11–12 % to 11.5–13 % under different loads on the unit. That is, the introduction of a control system with a model can increase the volume of ammonia up to 1.1 times, and, accordingly, reduce its cost by 10 %.

7. Conclusions

1. Analysis of the technological process as a control object, with the development of an information and logical scheme is the first stage of an integrated approach to the automation of complex technological processes. This is due to the fact that its results determine the possibility of using the technological reserve through more efficient use of raw materials, energy resources, reconstruction, and modernization of production. This is necessary to improve the efficiency of technological processes, including control systems. This problem is solved by reducing energy and resource costs.

2. Mathematical models have been built, including direct and inverse mathematical models of control objects. A feature of this development is the use of a combined form of mathematical models, which allows using a wider information base to obtain adequate mathematical models.

3. It is shown that at the stage of development of the control system with the model there should be structural and schematic diagrams of the control system, the calculated parameters of the system are determined and a set of technical means for the implementation of the system is selected.

4. The development of algorithms for the operation of the control system with the model involves the development of mathematical models of control objects and control principles, which are combined into a single algorithm for the functioning of the system.

5. At the stage of implementation and configuration of control systems with a model in accordance with the conditions of a particular production, a set of measures is developed for installation, commissioning, operation, maintenance, and possible modernization.

Conflicts of interest

The authors declare that they have no conflicts of interest in relation to the current study, including financial, personal, authorship, or any other, that could affect the study and the results reported in this paper.

Funding

The study was conducted without financial support.

Data availability

All data are available in the main text of the manuscript.

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