Computer Simulation System for Controlling Multiassortment Production of Sorption-catalytic Materials with Recycling of Returnable Waste

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***Abstract*—The article presents the structure of a computer system for modeling the processes of obtaining sorbents and catalysts. The core of the computer system is a library of deterministic and empirical mathematical models of the key stages of production (granulating, drying, tempering, and impregnation). Based on the models, the system allows solving the problem of resource-saving control of multi-assortment production in various modes of operation: when reconfiguring to a new type of product, in the nominal mode of operation, when a defect occurs. The use of the system by management and production personnel in the mode of an adviser to the operator-technologist allows increasing productivity and quality of products, reducing defective products and returnable waste, and reducing the cost of conducting research and re-construction of flexible production. The testing of the computer system according to data of JSC Scientific Design and Technological Bureau "Kristall" (St. Petersburg) confirmed its operability. The system can be used in various industries of sorption-catalytic materials.**

Keywords—mathematical modeling, computer system, sorbents, catalysts, returnable waste

I. Introduction

In the modern conditions of the development of the environmental controlling system, chemical industry enterprises are aimed at creating waste-free, operationally and environmentally safe productions. Production facilities are equipped with reliable automated control systems, software complexes for modeling various technological processes and information and training systems for training managerial production personnel [1-3]. It is especially important to solve these issues for production chemical-technological lines that have a complex, flexible, multi-stage production structure [4]. Such productions include the synthesis of a wide range of sorption-catalytic materials.

The products of the considered multiassortment production are used in gas analytical equipment, air conditioning and environmental support systems. This determines exacting requirements for the quality of sorption-catalytic products [5-10]. Only in Russia there are more than 20 enterprises producing sorption-catalytic materials for gas purification with a production capacity of 1-5 thousand tons per year [1, 4].

The complexity of controlling and studying the properties of various types of sorption-catalytic materials is due to the presence of uncontrolled disturbances (impurities in raw materials), the high cost of raw materials, sensitivity to the occurrence of defects when choosing control actions, the variety of physical and chemical processes for raw materials processing [5, 11-13]. Therefore, the task of creating a computer simulation system for controlling sorption-catalytic materials production with recycling of returnable waste is relevant and practical justified.

The computer system allows, based on mathematical models (MM) of key stages, to solve the problem of reconfiguring multi-assortment production to a new type of product, to issue recommendations on the choice of controlling influences at the production stages to ensure the required quality of intermediates and finished products, to conduct research on the operational properties of sorbents and catalysts, taking into account the analysis of the causes of violations of the structural strength and phase characteristics of materials, as well as the possibility of returning defective intermediates to previous production stages for further development.

II. Formulation of The Problem of Resource-Saving Control of The Sorption-Catalytic Materials Production

As an object of control, the process of obtaining sorbents and catalysts is characterized by: the production of various types of products $O = \{O_1, \ldots, O_z\}$ extensive nomenclature $N = \{N_1, \ldots, N_y\}$, the variety of technological stages $K = \{K_1, \ldots, K_h\}$, equipment $L = \{L_1, \ldots, L_w\}$, the possibility of obtaining the same product from different types of raw materials $R = \{R_1, \ldots, R_v\}$ according to various recipes $Z = \{Z_1, \ldots, Z_u\}$, strict requirements for the quality of intermediates $I = \{I_1, \ldots, I_s\}$ and finished products $J = \{J_1, \ldots, J_q\}$, the occurrence of unnominal situations at the production stages $\{D_1, \ldots, D_n\}$, related to the violation of product quality indicators and the presence of returnable waste (small things, crumbs, lumps, granules of irregular shape and size, granules with low strength) [4]. In the above formalized description, the following designations are adopted: z – the number of product types (sorbent, catalyst, carrier); y – the number of items of the product nomenclature; h – the number of stages; w – equipment; v – types of raw materials; u – recipes; s – requirements for the quality of intermediates; q – requirements for the quality of finished products; n – unnominal situations.

Unnominal situations include violations of the structural-strength and crystal-chemical properties of granules, the size and shape of the granules, the requirements for quality indicators, controlled visually. Fig. 1 shows the general scheme of flexible multiassortment production of sorption-catalytic materials. Table 1 describes the technological stages and types of returnable waste with an indication of recycling.

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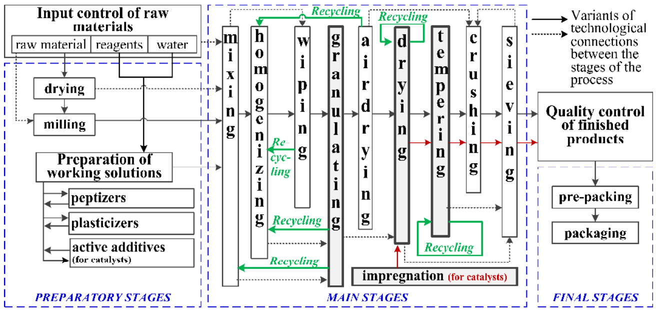

Fig. 1. General scheme of flexible multiassortment production of sorption-catalytic materials

TABLE I. TYPES OF RETURNABLE WASTE

Production stage	Type of defect (waste)	Recycling (return)	Controlled variables
Wiping	Clumping of granule embryos, clumping	Return to the homogenization stage	Homogenized mass moisture content W_{hg}
Granulating	Sticking of granular threads	Return to the mixing stage	Raw granules moisture content of W_0
	The content of small things, the presence of irregularly shaped granules	Return to the mixing stage	Plasticity η and the molding mass moisture content W_0
	Defects, cracks, burrs on the surface of the granules	Return to the homogenization stage	Plasticity of the mass η
	The output of granules of irregular shape	Return to the homogenization stage	Diameter of granules d
Air drying	Crushing of granules	Return to the homogenization stage	Granule wilt temperature T_{ad}
Drying	Substandard (underdried) granules	Return to the drying stage	Granules moisture content W
Tempering	Heterogeneity of the properties of granules	Return to the tempering stage	Mechanical strength P_m
	Violation of phase and structural-strength characteristics	Return to the tempering stage	Specific surface area S_p, total pore volume Vp, strength P_m

Fig. 2 shows a diagram of the relationship between the parameters of MM of the stages that have the greatest impact on the quality indicators of products, such as d – the diameter of the granules, m (at the granulation stage); V_p – total pore volume, m^3/kg; P_m – mechanical strength of granules, Pa; S_p – specific surface area, m^2/kg (at the stage of drying and tempering); ψ – uniformity of the solution distribution over the carrier granule (at the impregnation stage).

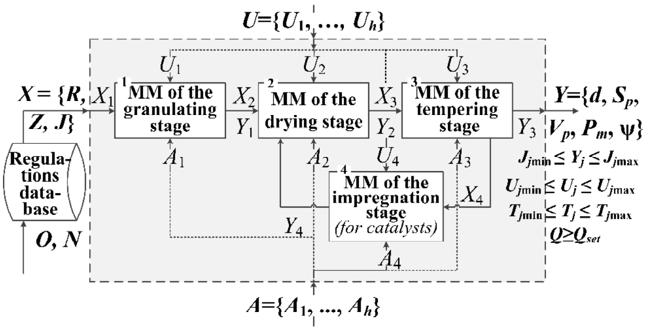

Fig. 2. Diagram of the relationship of the parameters of mathematical models of key stages of production

A generalized description of the basic deterministic and empirical MM should be presented in the form of a set of vectors $Y_j = f\{X_j, U_j, A_j, t\}$, where Y_j – vector of output variables, X_j – vector of input variables, U_j – vector of control actions, A_j – vector of coefficients of MM; t – simulation time; j – the index of belonging to the production stage.

Taking into account the proposed formalized description of the processes of obtaining sorbents and catalysts as an object of control and mathematical modeling, the problem of resource-saving control [4, 14] is formulated as follows:

1) To produce a certain type O and brand N of product, specified by the composition of raw materials R, recipe Z, to form a sequence of technological stages K, to determine the ranges of technological modes $[U_{jmin}; U_{jmax}]$ of equipment L to achieve a given line performance $Q \geq Q_{set}$ subject to restrictions on the quality of materials $J_{j\min} \leq Y_j \leq J_{j\max}$.

2) On the basis of the formed technological line K to determine the permissible control actions at each stage of production $U_j \in [U_{jmin}; U_{jmax}]$, providing the specified indicators of the quality of intermediates $I_{j\min} \leq Y_j \leq I_{j\max}$ and finished products $J_{j\min} \leq Y_j \leq J_{j\max}$.

3) In the event of a defect D, determine the most likely cause of a violation of the quality of materials $G = \{G_1, \ldots, G_l\}$, issue recommendations for controlling the process $B = \{B_1, \ldots, B_g\}$, determine the values of control actions to eliminate it $U_j \in [U_{jmin}; U_{jmax}]$, as well as the possibility of returning substandard granules to the previous stages of production.

III. FUNCTIONAL STRUCTURE OF A COMPUTER MODELING SYSTEM FOR CONTROLLING MULTIASSORTMENT PRODUCTION OF SORPTION-CATALYTIC MATERIALS

To solve the problem of resource-saving control of multiassortment production of sorption-catalytic materials with recycling of returnable waste, a functional structure of a computer system is proposed [4, 14], shown in Fig. 3.

The structure of the computer simulation system consists of: a databases of final products, quality requirements for sorbents and catalysts, recipes, raw materials, waste, stages, equipment; knowledge base of unnominal situations; a module for the synthesis of a technological scheme taking into account recyclable waste; library of deterministic and empirical MM of key stages, methods for solving systems of algebraic and differential equations; module for performing computational experiments; module for visualization of simulation results; user interfaces.

To systematize information about unnominal situations, the causes of their occurrence and recommendations for controlling in the computer system, a production-frame model of knowledge representation was used. The computer system dataware is configured for various types of products, equipment, requirements for productivity and energy consumption of production [15-17].

The software has an open modular architecture. This allows supplementing the functionality of the system through the interaction of various problem-oriented program modules. There are two types of users in the computer system: the system administrator and the user (researcher) – the operator-technologist.

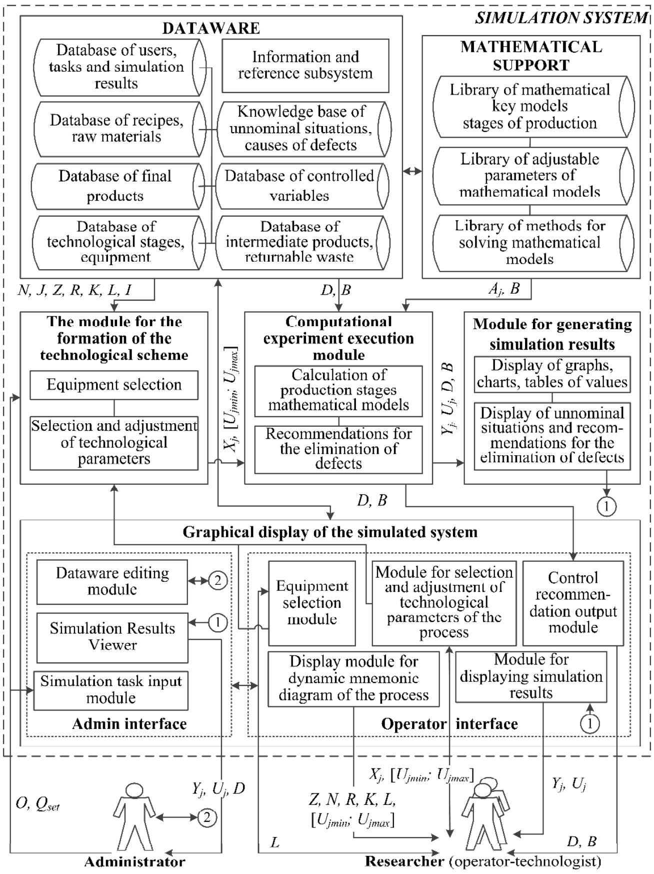

Fig. 3. The functional structure of the computer system

The computer system allows, in the mode of the operator's adviser, to issue recommendations to the user on controlling the processes of obtaining sorption-catalytic materials in the form of tables of values and two-dimensional and three-dimensional graphical dependencies of quality indicators on the values of control actions.

IV. Library of Mathematical Models of Key Stages of Sorption-Catalytic Materials Production

The library of MM of the key stages of production includes models of the granulating stage, thermal stages of drying and tempering, impregnation. The thermal stages of the process have the greatest influence on the formation of the structural-strength properties of the finished sorption-catalytic granules [4, 6, 7, 10].

At the drying stage, the water from acid solutions and molding water are removed from the granules, which are introduced into the composition of the granules when the molded mass is prepared at the mixing stage. During drying, there is a partial dehydration, solidification of the granules and their acquisition of high mechanical strength. The formalized description of the drying stage is presented in the form: $Y_2=f\{X_2, U_2, A_2, t\}$, where $X_2=\{X_{21}, X_{22}, X_{23}\}$, $X_{21}=\{T_{d0}, S, F_d, \}$ – variables that depend on the hardware implementation (T_{d0} – the initial air temperature in the drying chamber, ^{0}C; S – the area of the free evaporation surface, m^2; F_d – heat transfer surface area, m^2); $X_{22}=\{T_{20}, m_{wm}, V_{wm}, c_{wm}, W_0, W_{cr}, W_{eq},\}$ – variables characterizing the dried material (T_{20} – initial temperature of the material, ^{0}C; m_{wm} – material mass, kg; V_{wm} – the volume occupied by the wet material, m^3; c_{wm} – specific heat capacity, J/(kg·^{0}C); W_0, W_{cr}, W_{eq} – initial, critical, equilibrium material moisture content, %); $X_{23}=\{m_d, c_d, r\}$ – status parameters (m_d – air mass, kg; c_d – air heat capacity, J/(kg·^{0}C); r – specific heat of evaporation of moisture, J / kg); $U_2 = \{\tau, P\}$, where τ – drying time, s; P – power of the electric cabinet, W; $A_2=\{\alpha, \beta\}$, where α – heat transfer coefficient, W/(m^2·^{0}C); β – mass transfer coefficient, m/s; $Y_2=\{W, T_d, T_2\}$, where W – material moisture content, %; T_d – air temperature in the drying chamber, ^{0}C; T_2 – material temperature, ^{0}C.

The MM of the process of drying granules includes:

equations of the material balance in terms of product moisture content

$$dW/d\tau = -\beta S/V_{wm} \cdot (W - W_d)\,; \qquad (1)$$

the heat balance equation for the heat carrier (air)

$$d(T_d m_d c_d)/d\tau = P - \alpha F_d (T_d - T_2)\,; \qquad (2)$$

the heat balance equation for the material

$$d(T_2 m_{wm} c_{wm})/d\tau = \alpha F_d (T_d - T_2) - \\ - r m_{wm} \beta S/V_{wm} (W - W_d)/100 \qquad (3)$$

Initial conditions for the first period (the drying rate is constant and does not depend on the material moisture content) $\tau_0 = 0$; $T_d(\tau_0) = T_{d0}$; $T_2(\tau_0) = T_{20}$; $W(\tau_0) = W_0$; $W(\tau_{cr}) = W_{cr}$; $W_d = W_{cr}$; for the second drying period (the period of decreasing speed, at which the process is limited by the mass conductivity inside the wet material) $\tau_0 = \tau_{cr}$; $T_d(\tau_0) = T_{dcr}$, T_{dcr} – the initial air temperature in the drying chamber during the second drying period, ^{0}C; $T_2(\tau_0) = T_{2cr}$, T_{2cr} – the initial temperature of the material in the second drying period, ^{0}C; $W(\tau_0) = W_{cr}$; $W(\tau_{eq}) = W_{eq}$; $W_d = W_{eq}$.

The tempering stage determines the final strength, structural, sorption and catalytic properties of the finished granules. At the tempering stage, the components of the granules are decomposed and the crystal structure of the material is changed. The formalized description of the tempering stage is presented in the form: $Y_3=f\{X_3, U_3, A_3, t\}$, where $X_3=\{X_{31}, X_{32}, X_{33}\}$, $X_{31}=\{T_{p0}, P_p, F_t\}$ – variables that depend on the hardware implementation (T_p – calcination temperature, ^{0}C; P_p – muffle furnace power, W; F_t – heat transfer surface area, m^2); $X_{32}=\{V_{mt}, m_{mt}, c_{mt}, T_{30}, C_i^0\}$ – variables that characterize the material (V_{mt} – the volume occupied by the material, m^3; m_{mt} – mass of the material, kg; c_{mt} – specific heat capacity, J/(kg·^{0}C); T_{30} – initial temperature of the material, ^{0}C; C_i^0 – the initial concentration of the i-th component, mol/m^3); $X_{33}=\{m_{am}, c_{ah}\}$ – status parameters, where m_{am} – air mass, kg; c_{ah} – air heat capacity, J/(kg·^{0}C); $U_3=\{\tau_p, T_p\}$, where τ_p – tempering time, s; T_p – tempering temperature, ^{0}C; $A_3=\{k_0, E, Hr, M\}$, where k_0 – pre-exponential factor for calculating the reaction rate constant k_1, m^3/(mol·s); E – activation energy, J/mol; Hr – thermal effect of the reaction, J/mol; $M=\{a_{01}, a_{11}, a_{02}, a_{12}, a_{22}, a_{03}, b_{01}, b_{11}, b_{21}, b_{02}, b_{12}, b_{22}, b_{03}, c_{01}, c_{11}, c_{21}, c_{02}, c_{12}, c_{22}, c_{03}\}$ – vector of empirical coefficients; $Y_3=\{S_p, V_p, P_m\}$, where S_p – specific surface area, m^2/kg; V_p – total pore volume, m^3/kg; P_m – mechanical strength, Pa.

The MM of the tempering process contains:

equations for determining the quality of sorbents and catalysts

$$V_p = b_{03}(b_{01} + b_{11}t + b_{21}t^2)(b_{02} + b_{12}T_p + b_{22}T_p{}^2), \quad (4)$$

$$P_m = c_{03}(c_{01} + c_{11}t + c_{21}t^2)(c_{02} + c_{12}T_p + c_{22}T_p{}^2), \quad (5)$$

for sorbents

$$S_p^s = a_{03}(a_{01} + a_{11}t)(a_{02} + a_{12}T_p), \quad (6)$$

for catalysts

$$S_p^c = a_{03}(a_{01} + a_{11}t)(a_{02} + a_{12} \cdot T_p + a_{22}T_p{}^2)\ ; \quad (7)$$

equations for determining the ambient T_p and material T_3 temperatures

$$d(T_p m_{am} c_{ah})/dt = P_p - \alpha_p F_t (T_p - T_3)\ ; \quad (8)$$

$$d(T_3 m_{mt} c_{mt})/dt = \alpha_p F_t (T_p - T_3) - wV_{mt} Hr\ . \quad (9)$$

Example of a decomposition reaction at the tempering stage for aluminum oxide catalysts:

$$2Al(OH)_3 \xrightarrow{k_1} Al_2O_3 + 3H_2O\ .$$

Equations for determining the rates of change in the concentrations of substances involved in the reaction:

$$w = k_1 C^2{}_{Al(OH)_3}\ ;\ dC_{Al(OH)_3}/dt = -2w\ ; \quad (10)$$
$$k_1 = k_0 \exp[-E/(R(T_p + 273))]$$

Initial conditions: when τ_{p0}=0; $C_i(\tau_{p0})=C_i^0$; $T_p(\tau_{p0})=T_{p0}$; $T_3(\tau_{p0})=T_{30}$, $0<t\le\tau_p$.

The Runge-Kutta method of the fourth order of accuracy is used to solve MM of the drying (1)-(3) and tempering (4)-(10) stages. MM are adaptive to the final products, raw materials and hardware design of the process. The adequacy of MM has been verified for various types of aluminum oxide sorption-catalytic materials: aluminum phosphate sorbent AF and aluminum-chromium phosphate catalyst AHF. The adequacy is confirmed by the fulfillment of the adequacy condition according to the Fisher criterion $F > F_{0,95}^{table}$, $F = S_{av}^2 / S_R^2$.

V. Results of Testing and Practical Implementation of The Computer System

The conducted testing of a computer system for resource-saving control of multi-assortment production of aluminum oxide sorption-catalytic materials (z = 2; y = 13; h = 15; w = 48; v = 7; u = 16; s =9; q =10; n = 55) confirmed its operability and the possibility of using it in the mode of an adviser to an operator-technologist at industrial enterprises. Examples of the initial data for testing a computer system are given in Table. 2.

TABLE II. Initial Data for Testing The System

Stage	Material	Material parameters	Technological parameters
Drying	AF, AHF	W_0=40%; T_{20}=200°C; $d=5\cdot10^{-3}$m; m_{wm0}=47,5kg	0≤τ≤21600 s, 1000≤P≤2250 W
Tempering	AF	C_{HNO3}=1,2 %mass., C_{P2O5}=7,0 %mass.	0≤τ_p≤18000 c, 400≤T_p≤800 0C, P_p=4000 W
	AHF	C_{HNO3}=0,4 %mass., C_{P2O5}=7,0 %mass.; C_{Cr2O3}=10,0 %mass.	0≤τ_p≤18000 c, 200≤T_p≤600 0C, P_p=3200 W

The results of calculating the systems of equations of MM are shown in Fig. 4, Fig. 5, Fig 6. Fig. 4 shows the results of calculating the MM of the drying stage, Fig. 5 shows the MM of the tempering stage. Fig. 6 shows an example of constructing the three-dimensional graphical dependence of mechanical strength on the time and temperature of tempering stage.

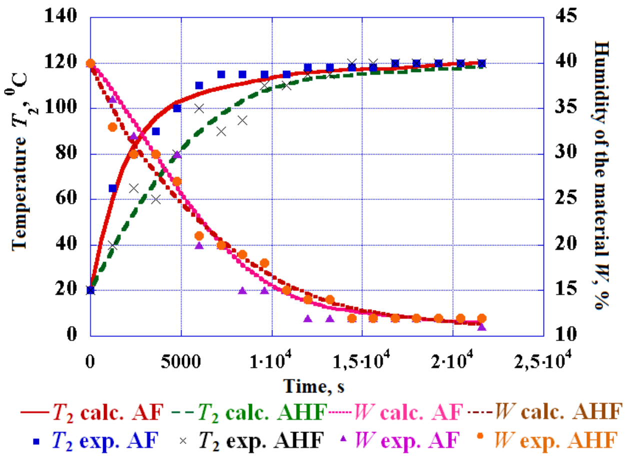

Fig. 4. Example of the results of calculating the system of equations of the model of the drying stage of aluminum oxide sorbents and catalysts

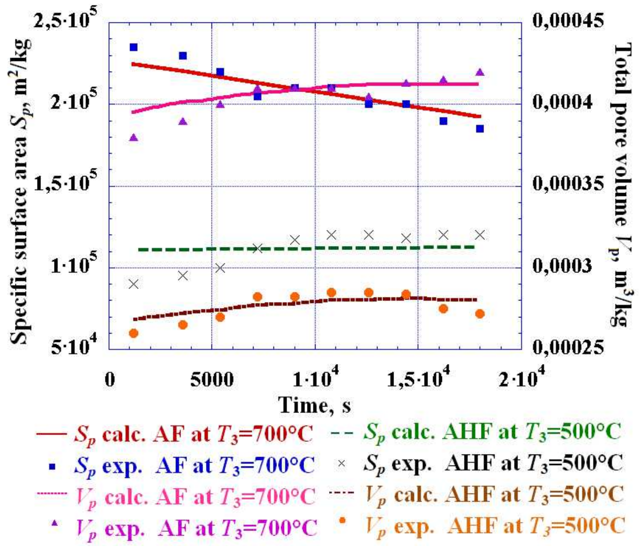

Fig. 5. Example of the results of calculating the system of equations of the tempering stage

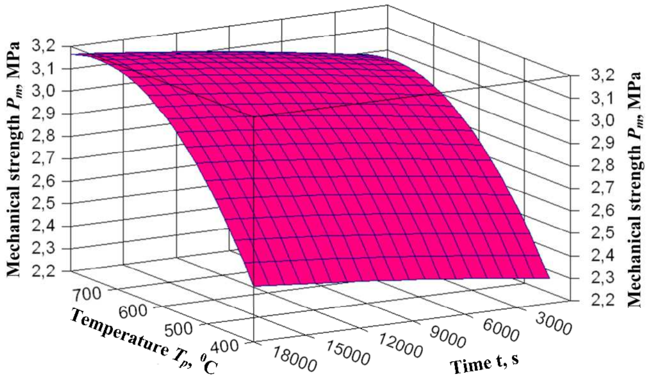

Fig. 6. Example of constructing a three-dimensional dependence of mechanical strength on the time and temperature of the tempering stage

According to the simulation results, the residence time of the material and the temperature at key stages of production have the greatest influence on the quality of sorption-catalytic materials. The results of testing and implementation of the computer system on the example of JSC Scientific Design and Technological Bureau "Kristall" (St. Petersburg) confirmed its operability and the possibility of using it to solve the problem of synthesis of a technological line, issuing control tips to achieve the required quality of production, as well as for training process operators to control the technological process in case of defects [3, 18].

VI. Conclusion

A comprehensive study of the flexible multiassortment production of sorption-catalytic materials with the processing of returnable waste was carried out. The analysis of production showed the need to develop a modular, adaptive architecture of a computer system that can be configured for various products, requirements for the quality of materials, hardware and technological design of processes. The structure of the computer system includes dataware, a module for forming a technological scheme of production with recycling of returnable waste, a module for calculating MM equations, a module for visualizing simulation results. The proposed MM of the key stages of the production of sorbents and catalysts allow us to investigate the laws of the main physical and chemical processes, evaluate the effectiveness of control at key stages of production, and solve the problem of reconfiguring production to a new type of production or the productivity of the technological line. The use of a computer system makes it possible to increase the efficiency of the production of sorption-catalytic materials by increasing the productivity and quality of products, reducing energy and material consumption, scrap and returnable waste, increasing environmental safety, reducing research costs. The computer system can be used as a training system to improve the professional level of managerial production personnel due to a deeper understanding of the cause-and-effect relationships of key process parameters and production control methods in the event of non-standard situations related to product defects and waste.

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